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POLARIZED RADIANCE. VOLUME II. POLARIZED SPECTRAL EMITTANCE FROM 4 TO 14 MICROMETERS

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Environmental Research Institute of Michigan

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Volume II of this report provides the Ballistic Research Laboratories with a description of a model for predicting emission polarization from paints. The report includes a description of measurements that were made along with graphs of measurement data. Validation of the model shows that model predictions agree with measurement to within the measurement accuracy 70% of the time, thus allowing degree of polarization to be calculated for smooth-surfaced materials in the thermal IR region for any λ (from about 7 to 15μm) and any polar angle, with

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Block 20. Abstract

only a measurement of spectral emittance from 7 to 15μm at any near-normal incidence required.

A listing of model parameters appropriate to the sample paints supplied ~~by BRL~~ is included along with a document explaining the use of the computer programs and listings of the programs as well.

FOREWORD

The work reported herein, covering the period 10 April 1972 to 31 December 1972, was carried out by the Infrared and Optics Division of the Environmental Research Institute of Michigan (formerly the Willow Run Laboratories of The University of Michigan), Ann Arbor, Michigan. The work was performed under Contract DAAD05-72-C-0216 for the Army Ballistic Research Laboratories, and was done in three parts, each of which represent one volume.

The three volumes are:

I - Polarized Bidirectional Reflectance With Lambertian or Non-Lambertian Diffuse Component.

II - Polarized Spectral Emittance From 4 to 14 μm.

III - Wavelength Dependence of Polarized Bidirectional Reflectance.

The internal number for volume II of this report is 192500-1-T(II)

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1. INTRODUCTION

Most materials on the earth's surface emit a large portion of their radiated energy in the thermal-infrared wavelength region. If irregularities of the surface of a natural target are very large compared to the wavelength of emitted radiation, total emissivity measurements are the prime source of information. However, if the surface irregularities of a target are small compared to the wavelength of emitted radiation, the surface tends to be more specular and the electric vectors of this emitted radiation will vibrate in preferential directions, giving rise to an observable emission polarization. For relatively smooth surfaces, therefore, polarization measurements are an additional source of information. Since the surfaces of military targets are generally smoother and have more ordered geometric patterns than naturally occurring materials, polarization is a potentially important parameter for target discrimination.

The purpose of this report is to describe a phenomenological model for predicting emission polarization of paints using as input only a single, near-normal reflectivity spectrum.

2. MODEL DESCRIPTION

For the case of an emitting polished surface, that portion of the emitted radiance at some angle θ to the target surface normal that has its electric vector vibrating perpendicular to the plane of emission (containing the surface normal and the propagation vector), divided by half the radiance emitted by a blackbody at the same temperature, is called the perpendicular component $E_{\perp}(\theta)$ of the emissivity. [Note: All the emissivity components are wavelength dependent, but the λ notation will be suppressed.] Likewise, the parallel emissivity component $E_{||}(\theta)$ defines that portion of radiation emitted with electric vector vibration parallel to the plane of emission. The total emissivity $E(\theta)$ is half the sum of $E_{\perp}(\theta)$ and $E_{||}(\theta)$.

The degree of polarization for emission can be defined as:

$$P_E = [E_{||}(\theta) - E_{\perp}(\theta)]/[E_{||}(\theta) + E_{\perp}(\theta)]. \quad (1)$$

The relationship between the emission polarization components and reflection polarization components can be found from a consideration of the reflection experiment where source (at θ_i) and observed (at θ_r) are located on opposite sides of the target surface normal at an angle $\theta = \theta_i = \theta_r$. Let $R_\perp$ and $R_{||}$ be the reflectivity components for radiation with electric vectors vibrating perpendicular and parallel, respectively, to the plane of incidence containing the incident and reflected rays. With the constraint that $\theta = \theta_i = \theta_r$, implying that the plane of emission coincides with the plane of incidence, Kirchhoff's law dictates (for equilibrium conditions) that

$$E(\theta)_\perp = 1 - R(\theta)_\perp, \quad (2a) \qquad E(\theta)_{||} = 1 - R(\theta)_{||}. \quad (2b)$$

The reflectivity flux components are functions only of $\theta_i = \theta_r = \theta$, and the complex index of refraction of the target material is given by $N = n - ik$. Expressions for $R_\perp$ and $R_{||}$ in terms of θ_e, n, and k are as follows [1]:

$$R_\perp(\theta) = \frac{[(a - \cos\theta)^2 + b^2]}{[(a + \cos\theta)^2 + b^2]} \tag{3a}$$

$$R_{||}(\theta) = \left\{\frac{[(a - \cos\theta)^2 + b^2]}{[(a + \cos\theta)^2 + b^2]}\right\} \times \left\{\frac{[(a - \sin\theta\tan\theta)^2 + b^2]}{[(a + \sin\theta\tan\theta)^2 + b^2]}\right\}, \tag{3b}$$

where

$$a^2 = \frac{1}{2}\{n^2 - k^2 - \sin^2\theta + [4n^2k^2 + (n^2 - k^2 - \sin^2\theta)^2]^{\frac{1}{2}}\}$$

and

$$b^2 = \frac{1}{2}\{-n^2 + k^2 + \sin^2\theta + [4n^2k^2 + (n^2 - k^2 - \sin^2\theta)^2]^{\frac{1}{2}}\}$$

From Eqs. (1), (2), and (3), therefore, it is possible to express the degree of emission polarization P_E as a function of θ, n, and k.

For materials which exhibit reststrahlen bands in the thermal-IR wavelength region, n and k are strongly wavelength-dependent in that region. The wavelength dependence of P_E for a given material can be calculated from Eqs. (1), (2), and (3) if the dispersion curves of n and k are known. Once these dispersion curves have been determined as continuous functions of wavelength for a given paint, it is then possible to calculate the emission polarization for all θ as a function of λ. This will be calculated for several O.D. paints.

One means for determining the indices of refraction is the classical oscillator fitting method. The complex index of refraction $N = n - ik$ can be calculated as a function of frequency ν, according to a classical oscillator model of crystals [2], from the following equations:

$$2nk = \sum_j 4\pi p_j \nu_j^2 \left[\frac{\gamma_j \nu_j \nu}{(\nu_j^2 - \nu^2)^2 + \gamma_j^2 \nu_j^2 \nu^2}\right],$$

$$n^2 - k^2 = \varepsilon_\infty + \sum_j 4\pi p_j \nu_j^2 \left[\frac{\nu_j^2 - \nu^2}{(\nu_j^2 - \nu^2)^2 + \gamma_j^2 \nu_j^2 \nu^2}\right], \qquad (4)$$

where p_j, γ_j, and ν_j are the strength, width, and frequency, respectively, of the j^{th} lattice oscillator and ε_∞ is the high frequency dielectric constant. If these oscillator parameters are known, n and k are calculable from Eq. (4). If they are unknown, they can be estimated by the following procedure. Initial guesses for the oscillator parameters are assumed, (see Appendix D) and a normal incidence Fresnel reflectivity curve $R(\nu)$ is calculated from the equation:

$$R(\nu) = \left\{\frac{[n(\nu) - 1]^2 + k^2(\nu)}{[n(\nu) + 1]^2 + k^2(\nu)}\right\} \qquad (5)$$

A computer program, which employs an IBM scientific subroutine, [see Appendix F] compares the theoretical reflectivity curve calculated from Eq. (5) with an experimental normal incidence spectral reflectivity curve for a smooth surface of the specimen, changes the oscillator parameters in Eq. (4), calculates a new theoretical curve, and reiterates until a good fit is made between theoretical and experimental curves. With the oscillator parameters of the best-fitting theoretical curve, the indices can then be calculated from Eq. (4). (See Appendix D for use of Oscillator Program.)

3. MEASUREMENTS

The measurements in this program consisted of two phases. The first phase consisted of a spectral scan of the emittance from each sample with a normal angle of observation. The second phase consisted of angular scans of the emittance with receiver polarizer set alternately perpendicular and parallel to the receiver incidence plane. In this latter case, each scan took place at a particular wavelength.

In the following paragraphs we provide a brief description of the instrument which was used for these measurements, followed by data which resulted.

3.1 The Instrument

The field infrared spectroradiometer (FISR) which was utilized is a double-beam instrument with output proportional to the radiance difference between the objects filling the fields of the two Herschelian reflecting telescopes. The measurement of the difference is accomplished by a reflective chopper which alternately samples the radiation from the two telescopes. After being chopped, the radiation from the two telesceopes is imaged at a common focal plane at which a field stop slit is placed, limiting the FOV to a 0.6' x 2.5° field. The fore-optics just described are illustrated in Figure 1. The chopped energy passing through the field stop slit is refocused, by a 90° off-axis ellipsoid mirror, onto an entrance aperture which lies immediately in front of the circular variable-filter (CVF) monochromator.

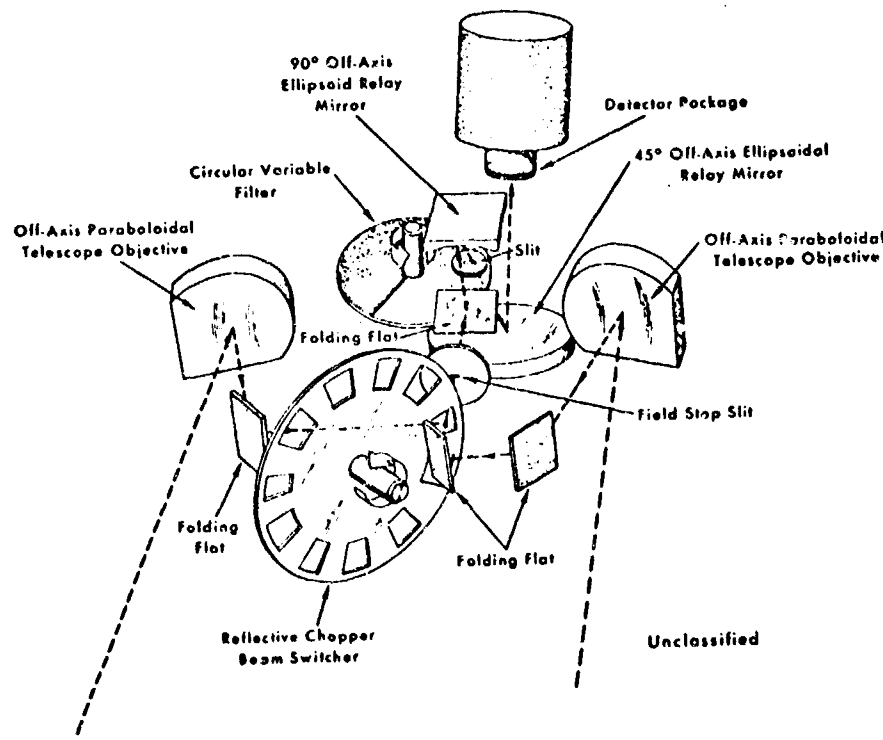


Figure 1. SCHEMATIC OF FI[illegible]R FORE-OPTICS

The CVF then transmits a narrow spectral band of this energy to a 45° off-axis ellipsoid mirror, which refocuses it onto the detector.

The generated ac detector signal is amplified and then synchronously demodulated. The synchronous demodulator transforms those components of the signal which have the particular frequency of the chopper modulation into a proportional dc signal, while rejecting those components with different frequency (i.e., noise). Thus, at the output a dc signal is presented which has a value at any point in time proportional to the energy difference between the two optical beams at a particular wavelength determined by the CVF position. Mechanical rotation of the CVF provides a spectral scan. The output voltage is recorded by using a digital voltmeter as an analog-to-digital converter and printing on a digital paper-tape printer, and the wavelength is registered simultaneously by printing the digital output of a shaft encoder mechanically linked to the CVF.

The spectrometer portion of the system utilized a circular variable filter for spectral dispersion in the range from 2.5 to 14.5μm. The CVF has the advantage of providing more efficient energy transmission than a prism disperser, allowing faster spectral scan rates or narrower spectral resolution for a given energy input.

In order to achieve high system sensitivity, an indium antimonide and a mercury doped germanium detector are used to cover the wavelength regions 2.5 to 5.5μm and 4.5 to 14.5μm, respectively. These detectors are readily interchangeable, so one may be replaced by the other during the course of scanning from 2.5 to 14.5μm without stopping the instrument.

Two temperature-controlled blackbody calibration sources are provided for insertion at the entrance optics in either or both of the two channels. In the normal mode of operation, a blackbody remains in one channel, and the other channel, having previously been calibrated, views the target of interest. In this way the system can be used to measure absolute radiance. Alternatively, if the target temperature is known, or if a black surface at the same temperature is available, the spectral emittance of the surfae can be determined. These blackbodies are only suitable for the spectral

range 4.5 to 14.5μm. Calibration sources below 4.5μm have not as yet been implemented. However, for these reflective wavelengths (less than 4.5μm), a calibrated reflectance panel may be inserted in the reference beam and the instrument then used to make relative reflectance measurements.

Supplementary instrumentation has been developed to permit the basic FISR equipment to be used for obtaining directional polarized emissivity data. Two similar samples maintained at different known temperatures are separately viewed through each port of the FISR, and the difference in radiance values is measured. From this measured difference, with the available temperature information, the emissivity can be calculated. The sample temperatures are maintained by thermally controlled water baths. The sample holder is designed to be operated either at a fixed viewing angle or by revolving and permitting a scan of the sample surface.

Complete details of the FISR can be found in reference 4.

3.2 Spectral Emittance

Figures 2, 3 and 4 show the spectral emittance data in plotted form. In each case there are many scans, some of which cover different spectral regions than others. Each scan number has its own symbol so it can be roughly identified on the plot. Shown also are curves representing both accuracy and precision of the measurements. Accuracy is determined with respect to both systematic and random errors. Precision is determined with respect to noise in the recorded voltage. (Reference 4 provides a complete discussion of determination of accuracy and precision in this context.)

Note that for all three samples, there is an apparent dip in the spectrum between 9.5μm and 10μm. This dip is interpreted to be a reststrahlen band. Structure of this sort arises from the wavelength dependence of the indices of refraction. (In section 1, we have described how one calculates the indices of refraction by use of a classical oscillator fitting method.)

Note also that in Figure 3 there is an apparent discrepancy in that scans numbers 3 and 4 are translated upward with respect to scans 2 and 23. This discrepancy appears to be due to a combination of calibration error and difficulty of maintaining accurate measurement of environment temperature during the measurements. The problem is still being analyzed. In the validation (see Section 4) scans 3 and 4 were used. In view of the apparent difficulty it is not clear that these were the most appropriate.

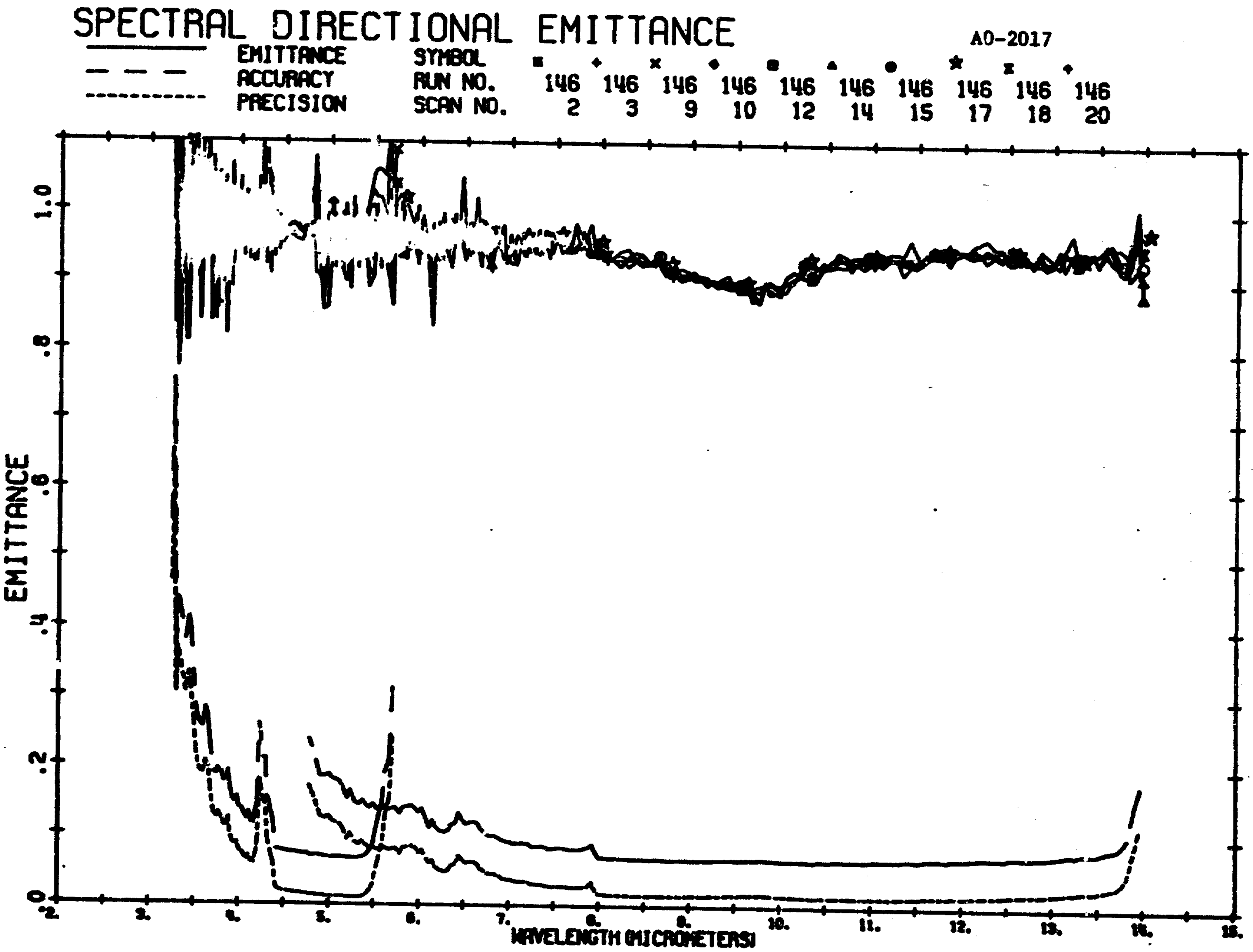
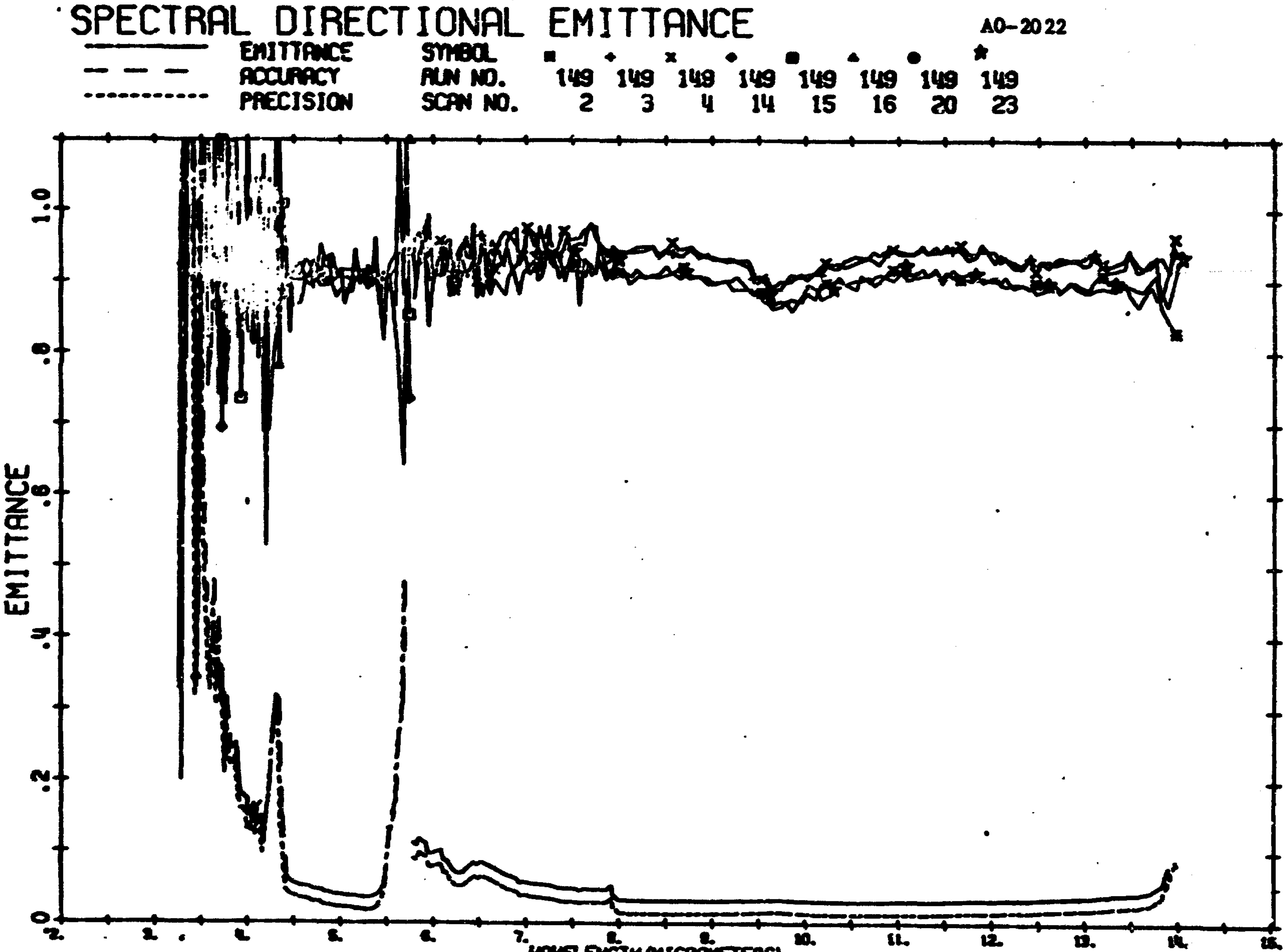

SPECTRAL DIRECTIONAL EMITTANCE
AO-2017
EMITTANCE
ACCURACY
PRECISION
SYMBOL
RUN NO. 146 146 146 146 146 146 146 146 146 146
SCAN NO. 2 3 9 10 12 14 15 17 18 20
EMITTANCE
0
.2
.4
.6
.8
1.0
WAVELENGTH (MICROMETERS)

FIGURE 2



SPECTRAL DIRECTIONAL EMITTANCE
AO-2022
EMITTANCE
ACCURACY
PRECISION
SYMBOL
RUN NO. 149 149 149 149 149 149 149 149
SCAN NO. 2 3 4 14 15 16 20 23
EMITTANCE
WAVELENGTH (MICROMETERS)

FIGURE 3

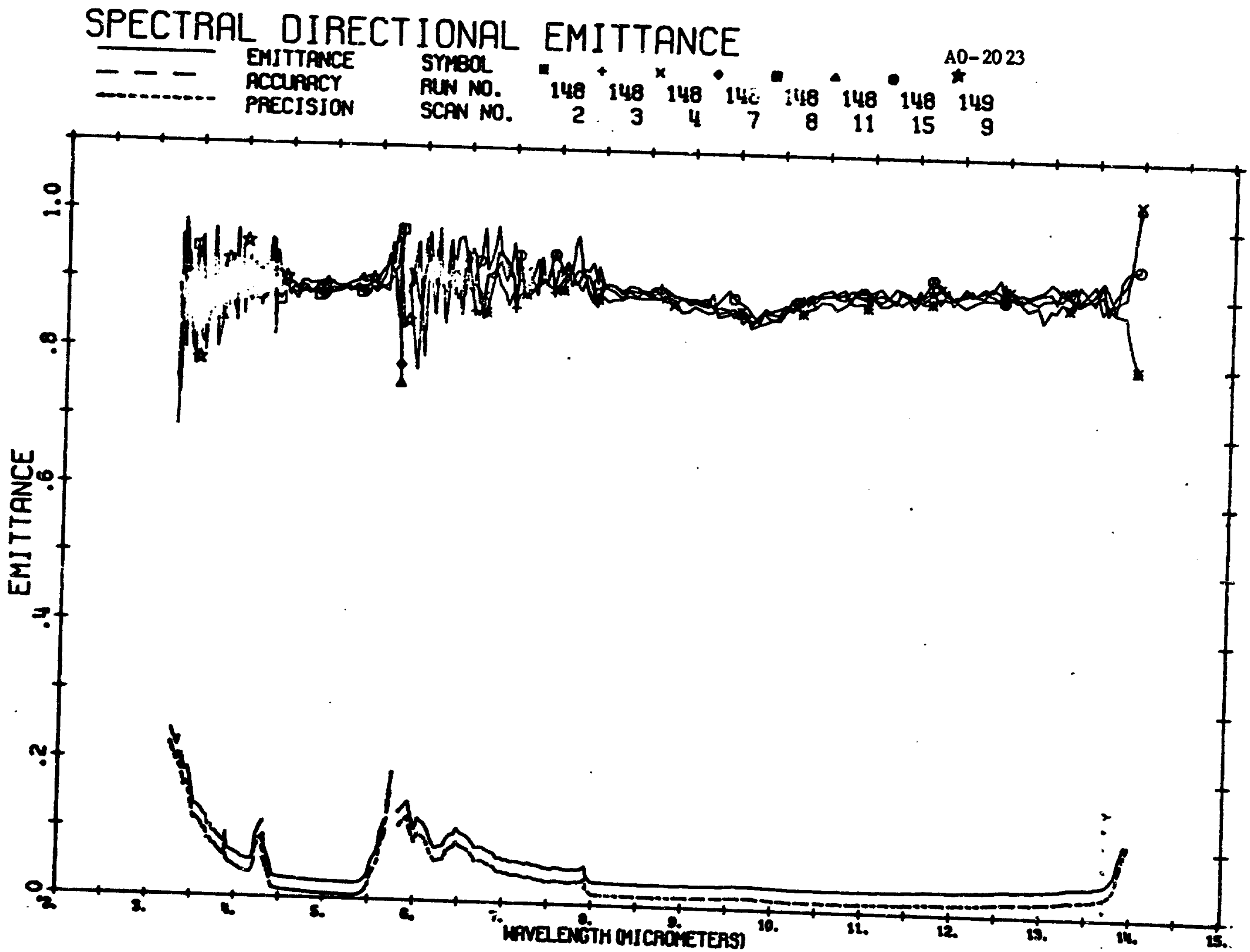

SPECTRAL DIRECTIONAL EMITTANCE
EMITTANCE
ACCURACY
PRECISION
SYMBOL
RUN NO. 148 148 148 148 148 148 148 149
SCAN NO. 2 3 4 7 8 11 15 9
AO-2023
EMITTANCE
1.0
.8
.6
.4
.2
0
2.
3.
4.
5.
6.
7.
8.
9.
10.
11.
12.
13.
14.
15.
WAVELENGTH (MICROMETERS)

FIGURE 4

3.3 <u>Polarized Emittance vs. Angle</u>

Figures 5 through 16 show the variation for each sample at a variety of wavelengths of relative polarized emittance. In each case the curve which represents parallel polarization is a plot of $e_{||}(\theta) = \frac{E_{||}(\theta)}{E_{||}(0)}$ and that which represents perpendicular polarization is $e_{\perp}(\theta) = \frac{E_{\perp}(\theta)}{E_{\perp}(0)}$.

Therefore, for each angle, degree of polarization is extracted from the data by equation (1), where substituting $e_{||}(\theta)$ and $e_{\perp}(\theta)$ for $E_{\perp}(\theta)$ and $E_{||}(\theta)$ leaves P_E unchanged, since $E_{||}(0) = E_{\perp}(0) = E(0)$. [See Appendix A]. Comparison of model predictions with selected measurement data from this group is described in Section 4.

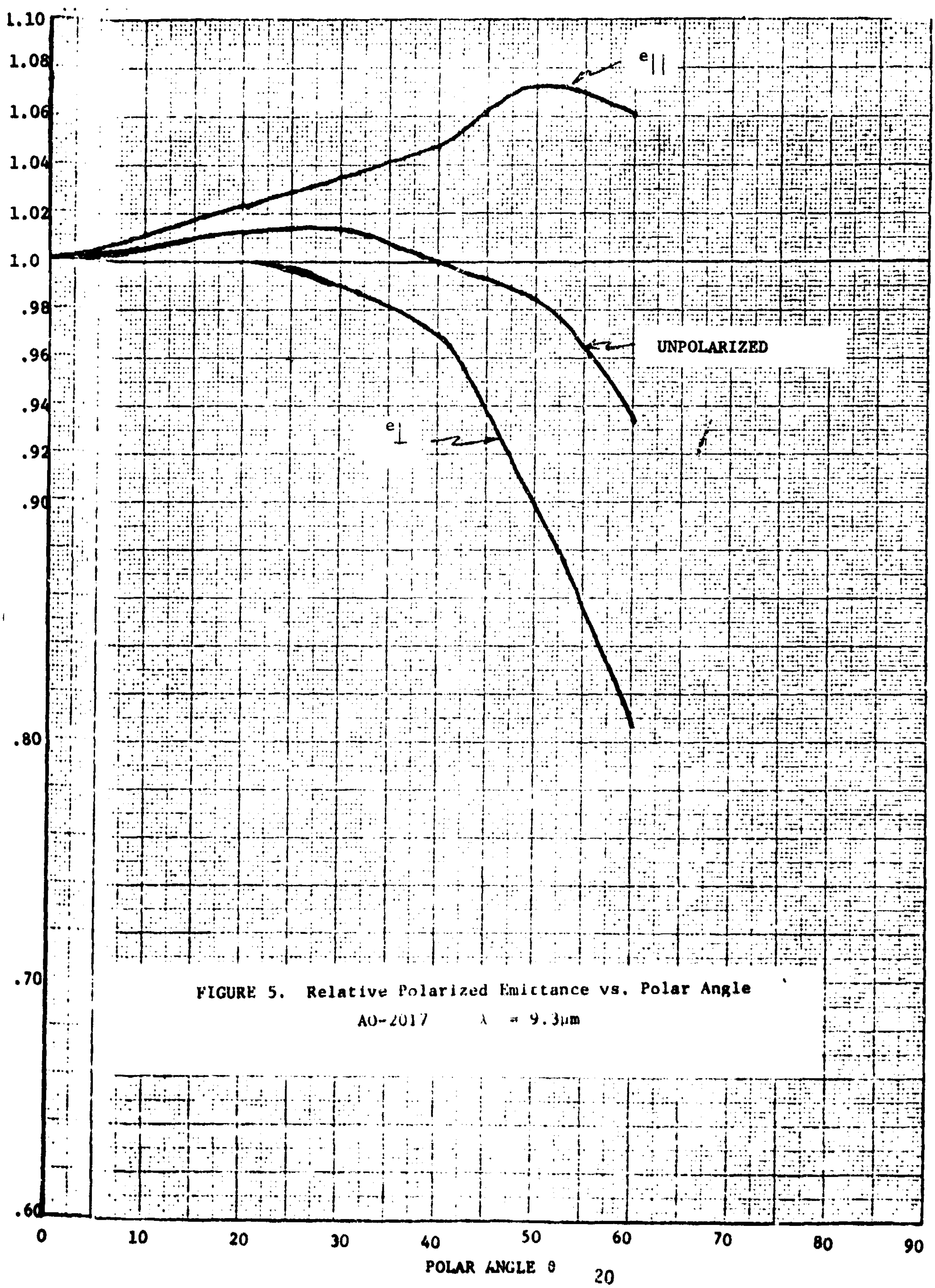


FIGURE 5. Relative Polarized Emittance vs. Polar Angle
AO-2017 λ = 9.3μm

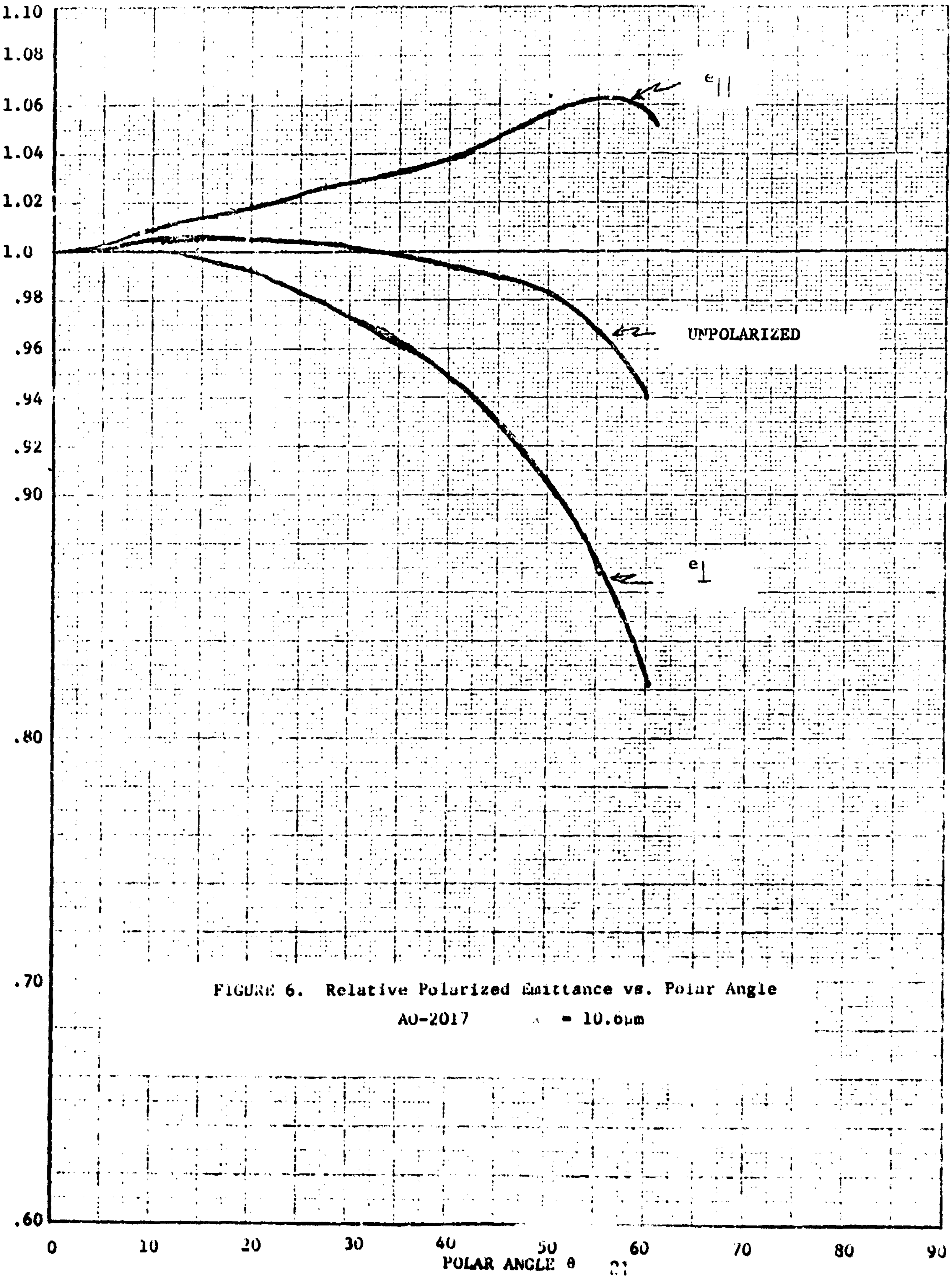


FIGURE 6. Relative Polarized Emittance vs. Polar Angle
AO-2017 λ = 10.6μm

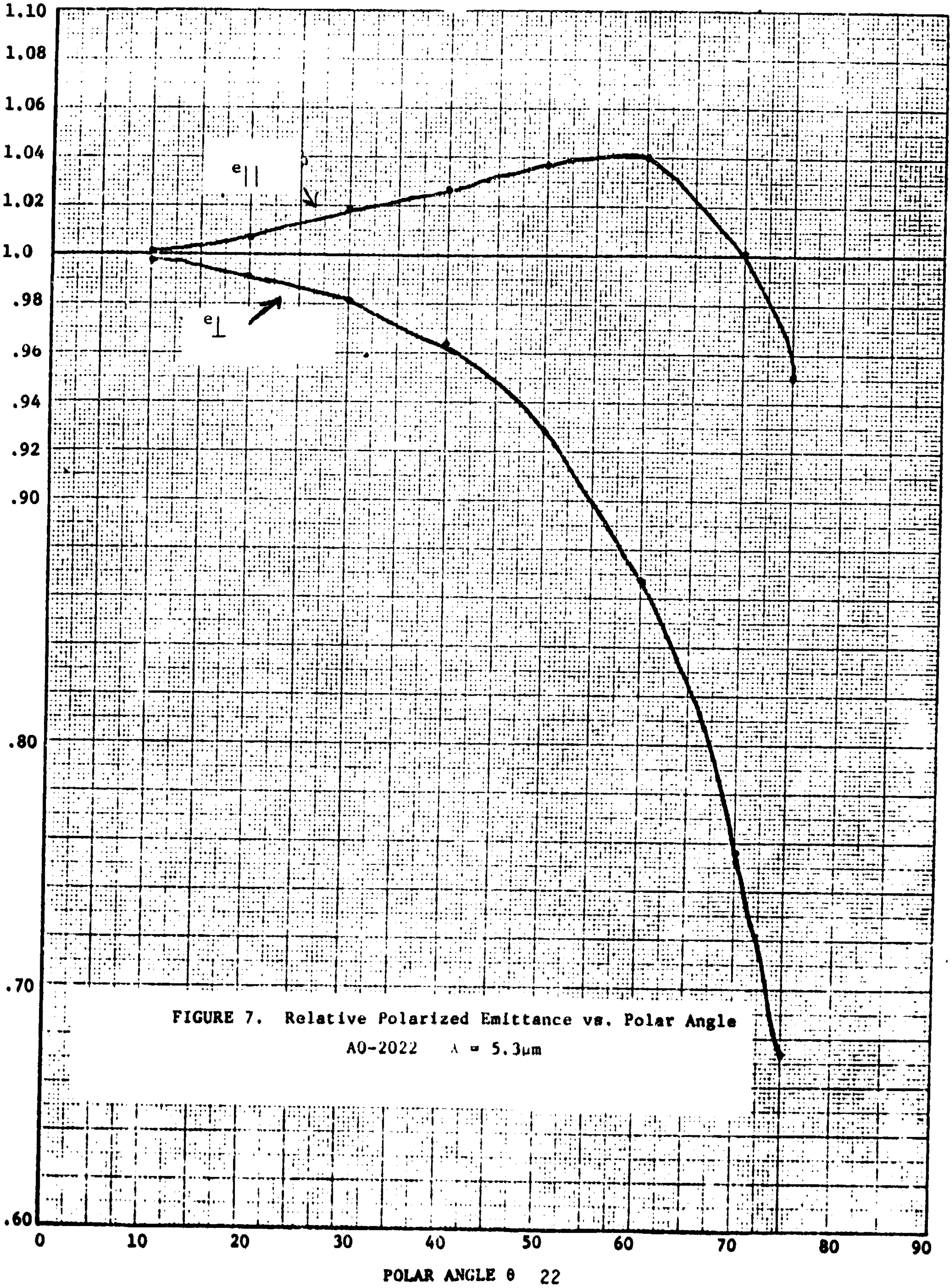


FIGURE 7. Relative Polarized Emittance vs. Polar Angle
A0-2022 λ = 5.3μm

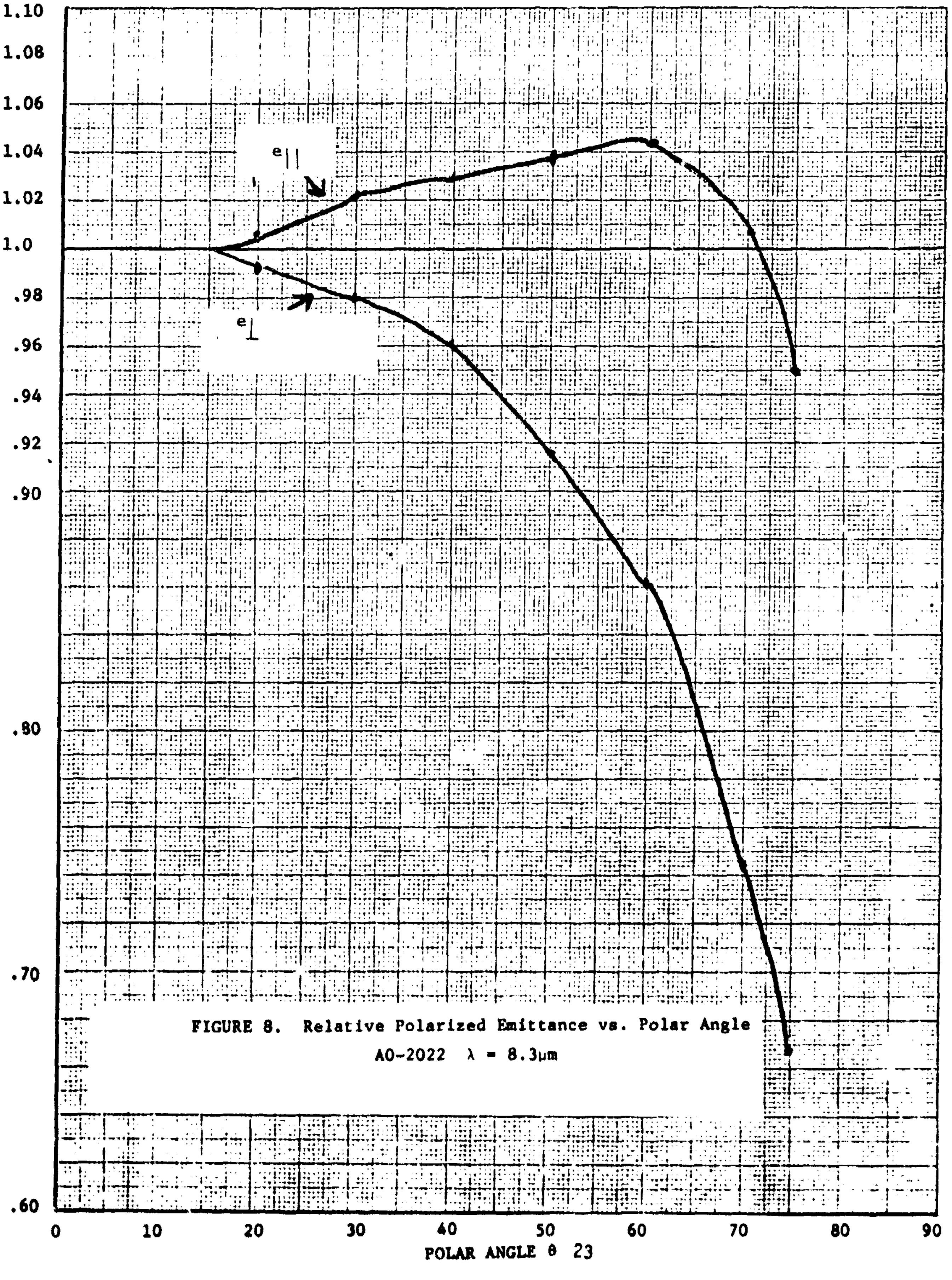


FIGURE 8. Relative Polarized Emittance vs. Polar Angle
AO-2022 λ = 8.3μm

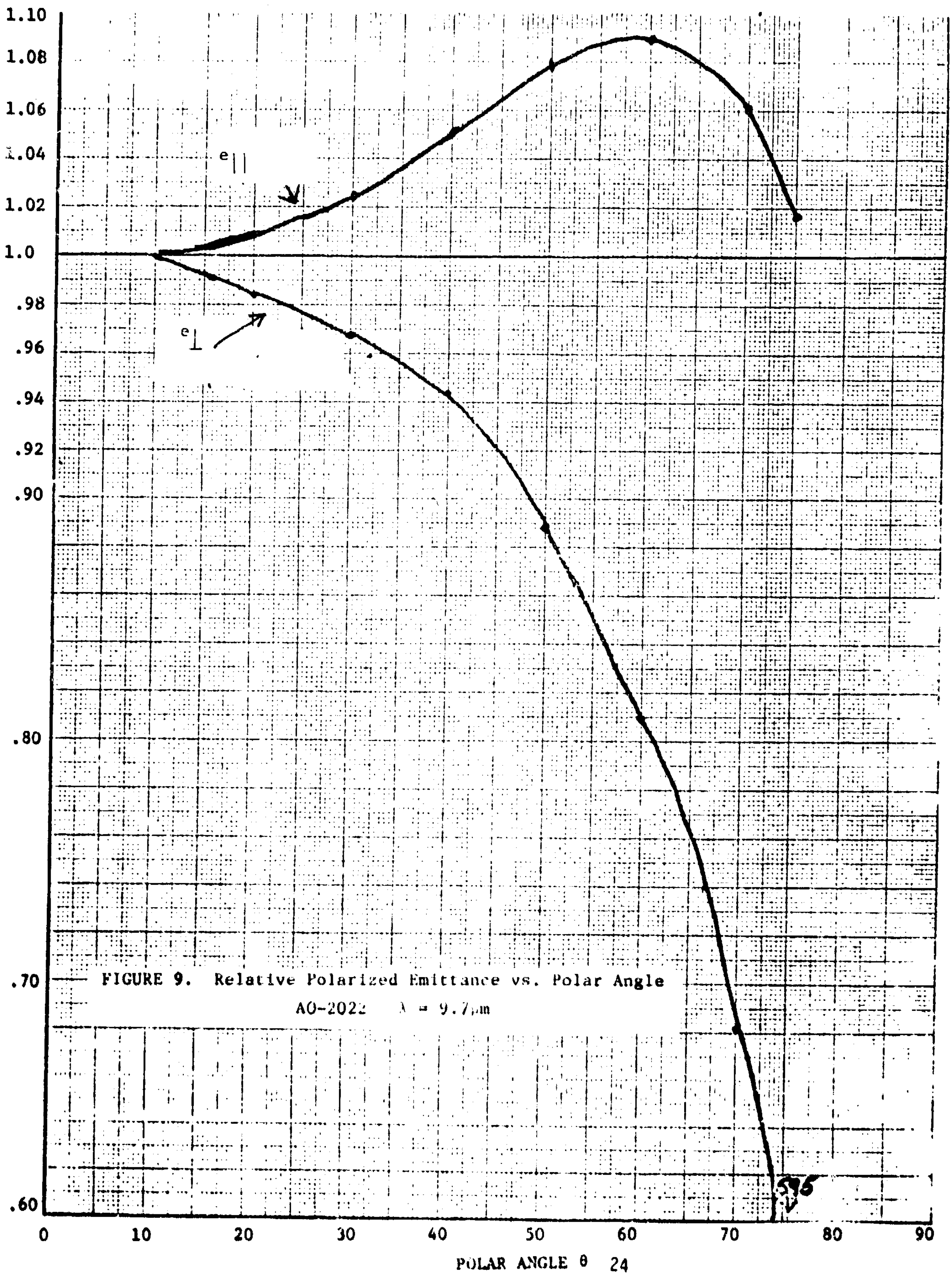


FIGURE 9. Relative Polarized Emittance vs. Polar Angle
AO-2022 λ = 9.7μm

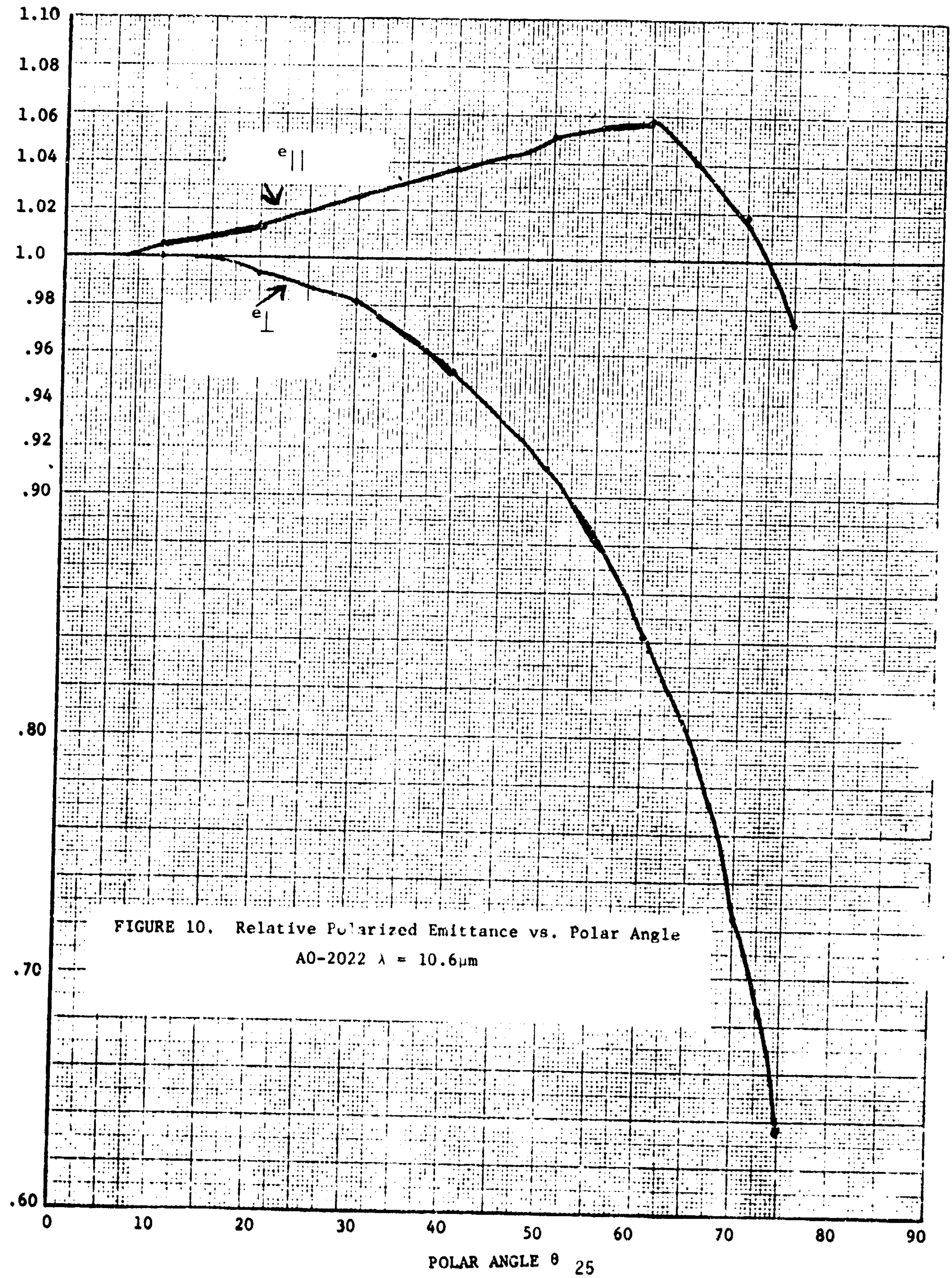


FIGURE 10. Relative Polarized Emittance vs. Polar Angle
A0-2022 $\lambda = 10.6\mu m$

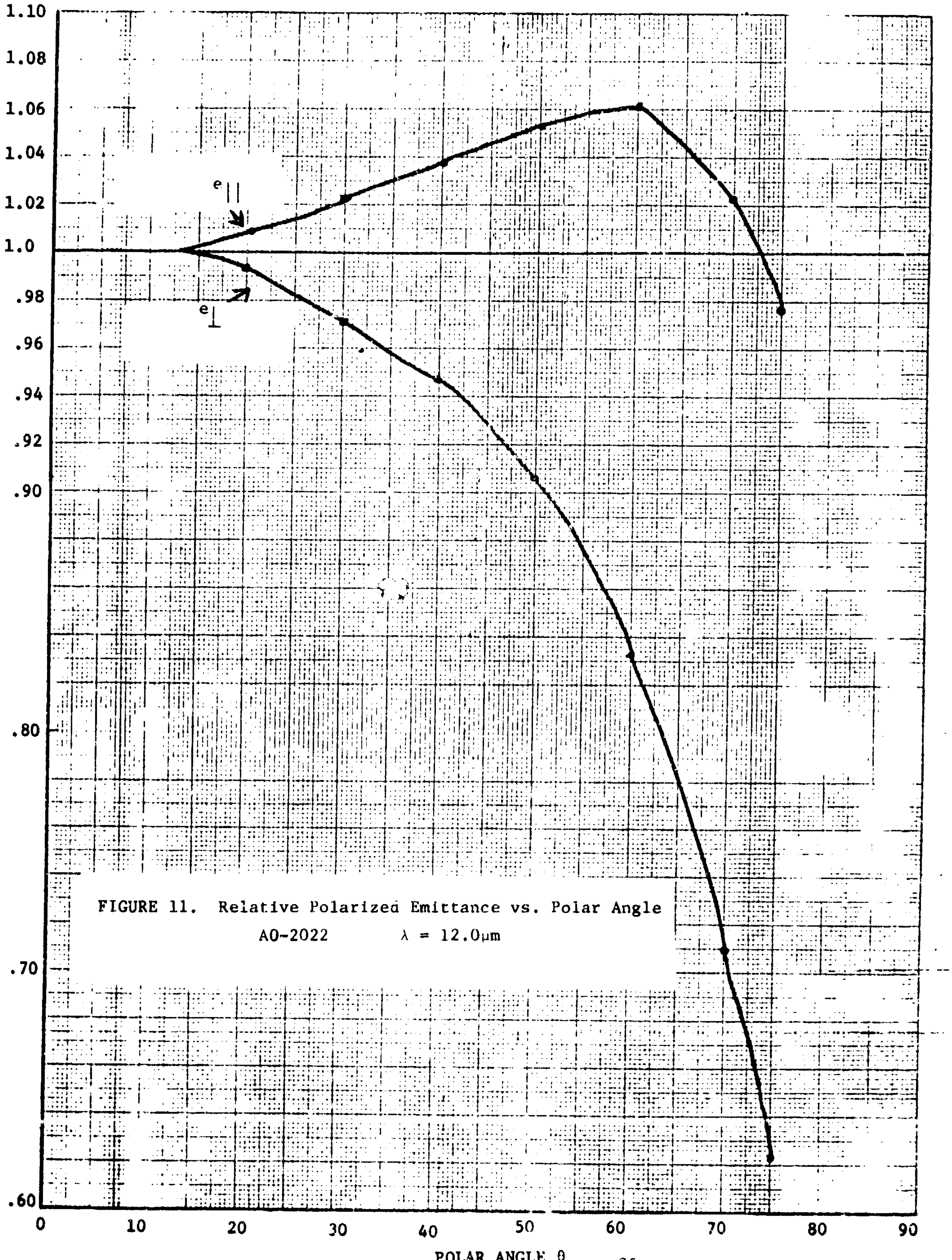


FIGURE 11. Relative Polarized Emittance vs. Polar Angle
A0-2022 λ = 12.0μm

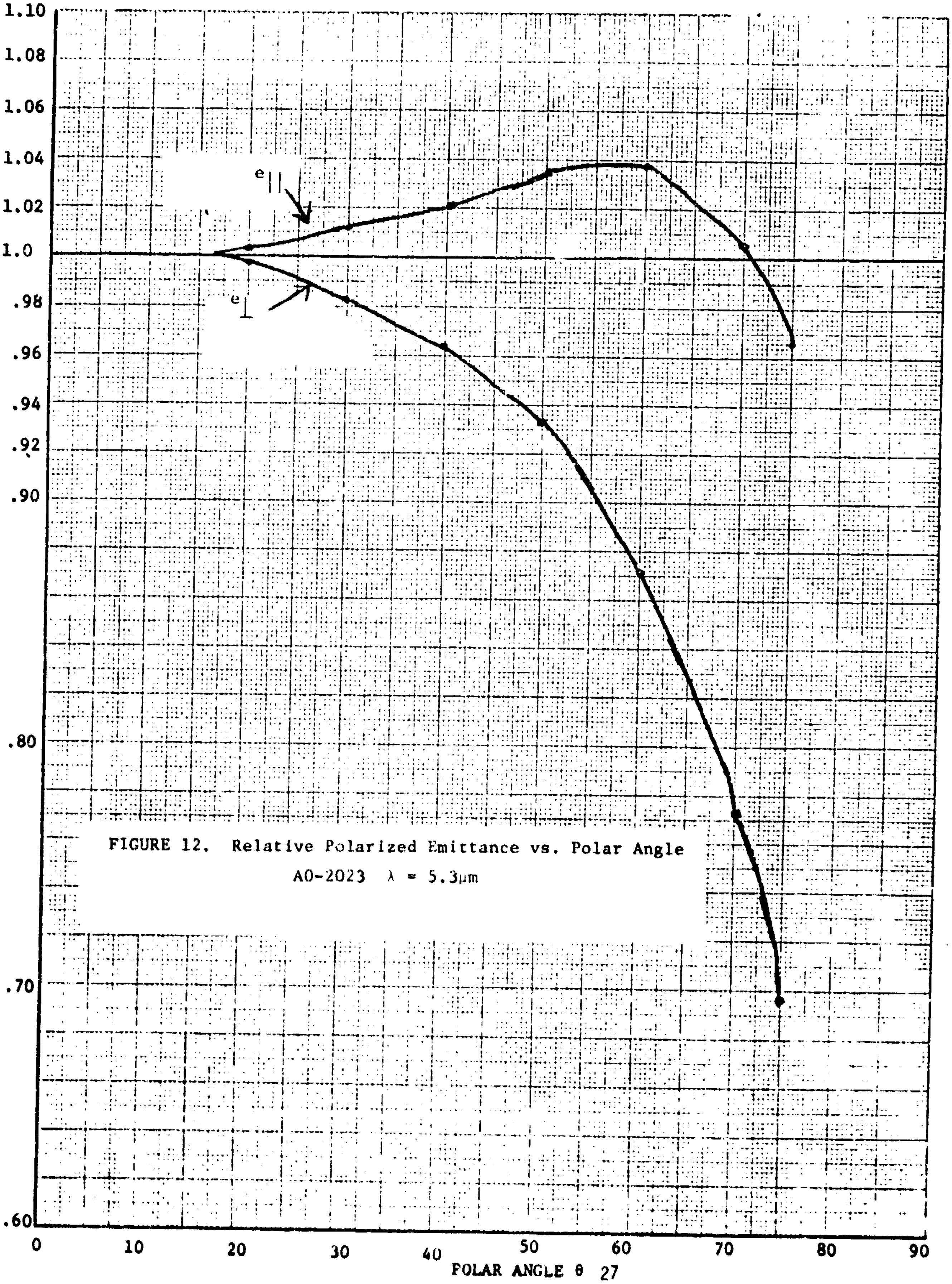


FIGURE 12. Relative Polarized Emittance vs. Polar Angle
A0-2023 $\lambda = 5.3\mu m$

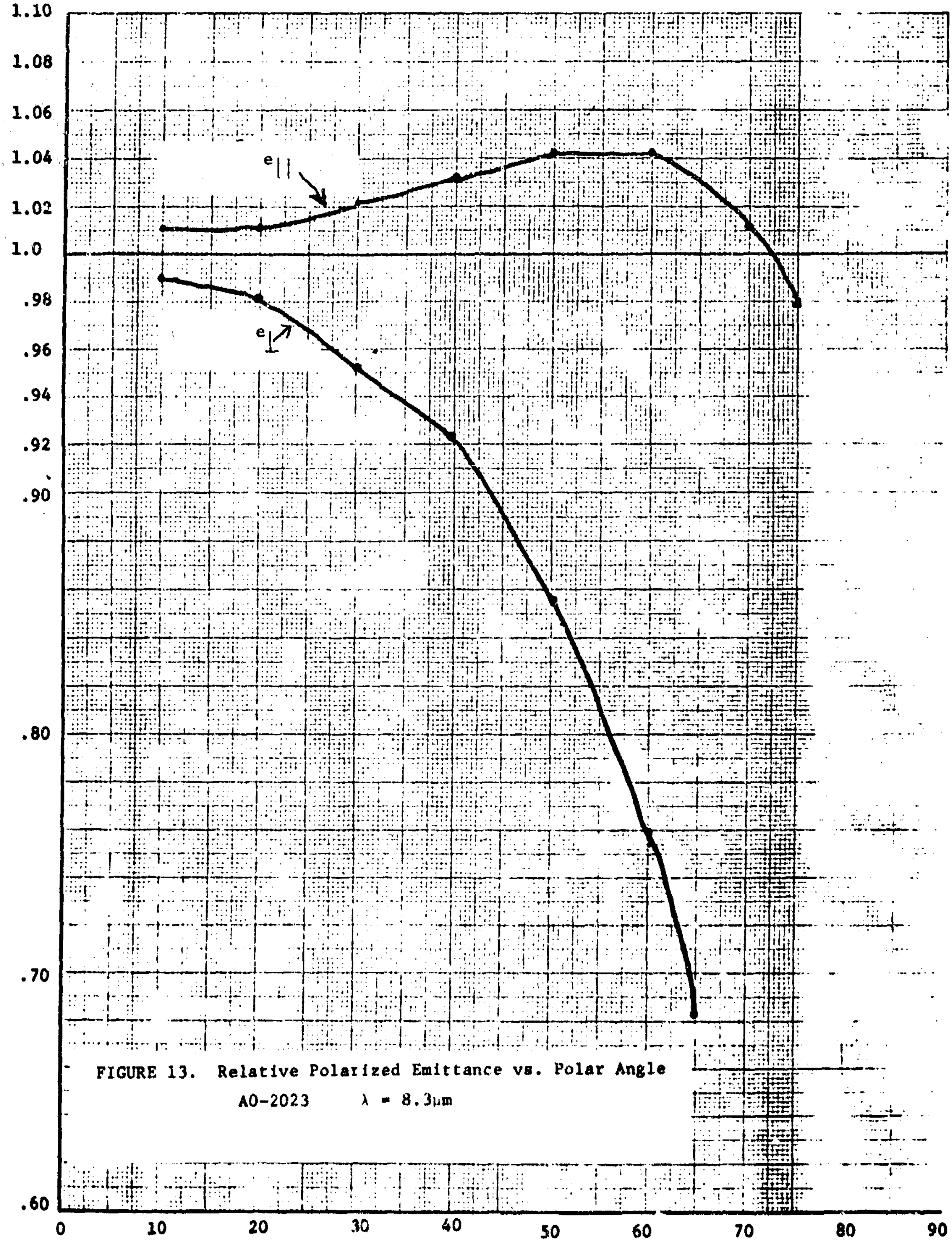


FIGURE 13. Relative Polarized Emittance vs. Polar Angle

A0-2023 λ = 8.3μm

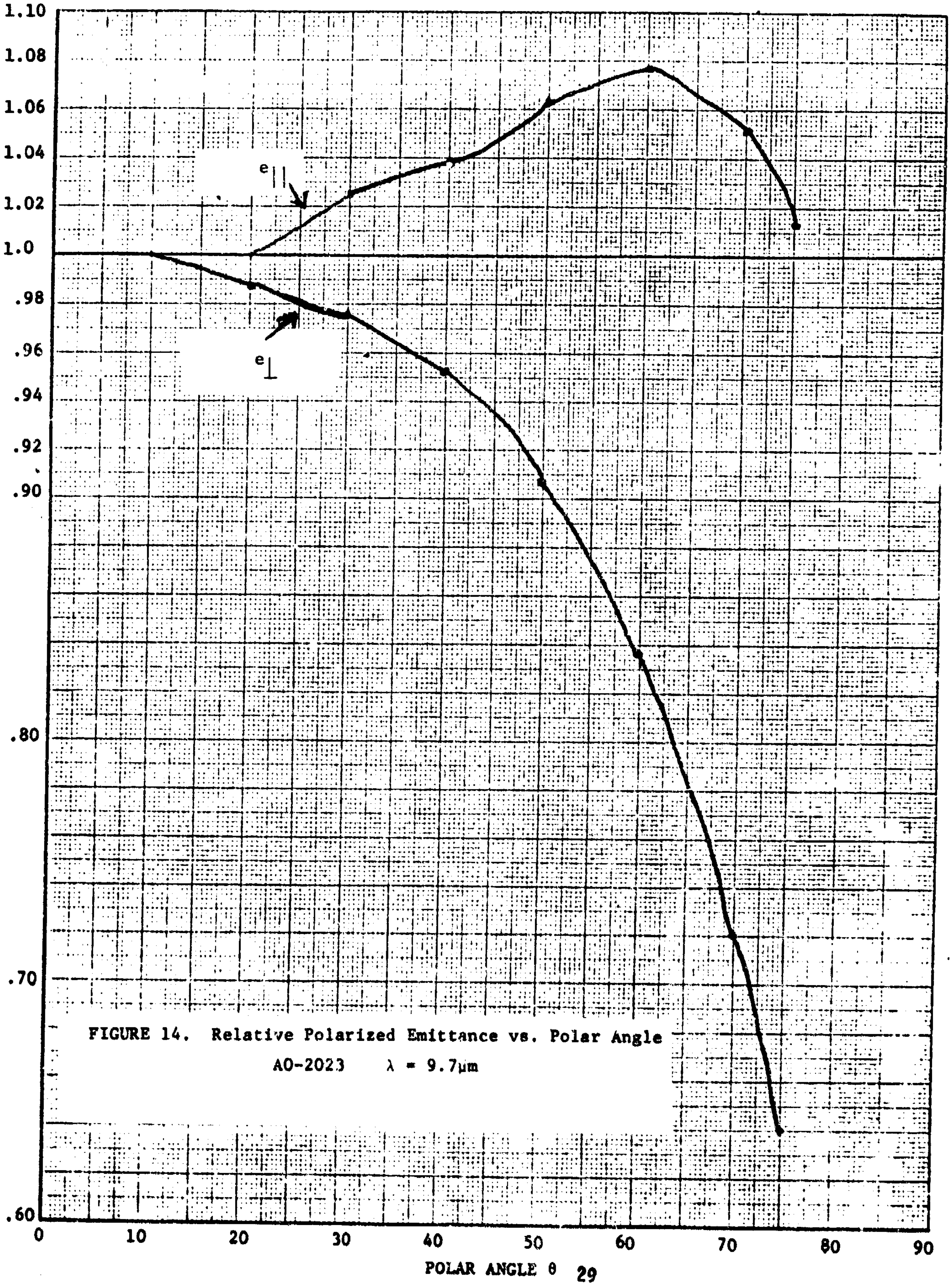


FIGURE 14. Relative Polarized Emittance vs. Polar Angle
AO-2023 $\lambda = 9.7\mu m$

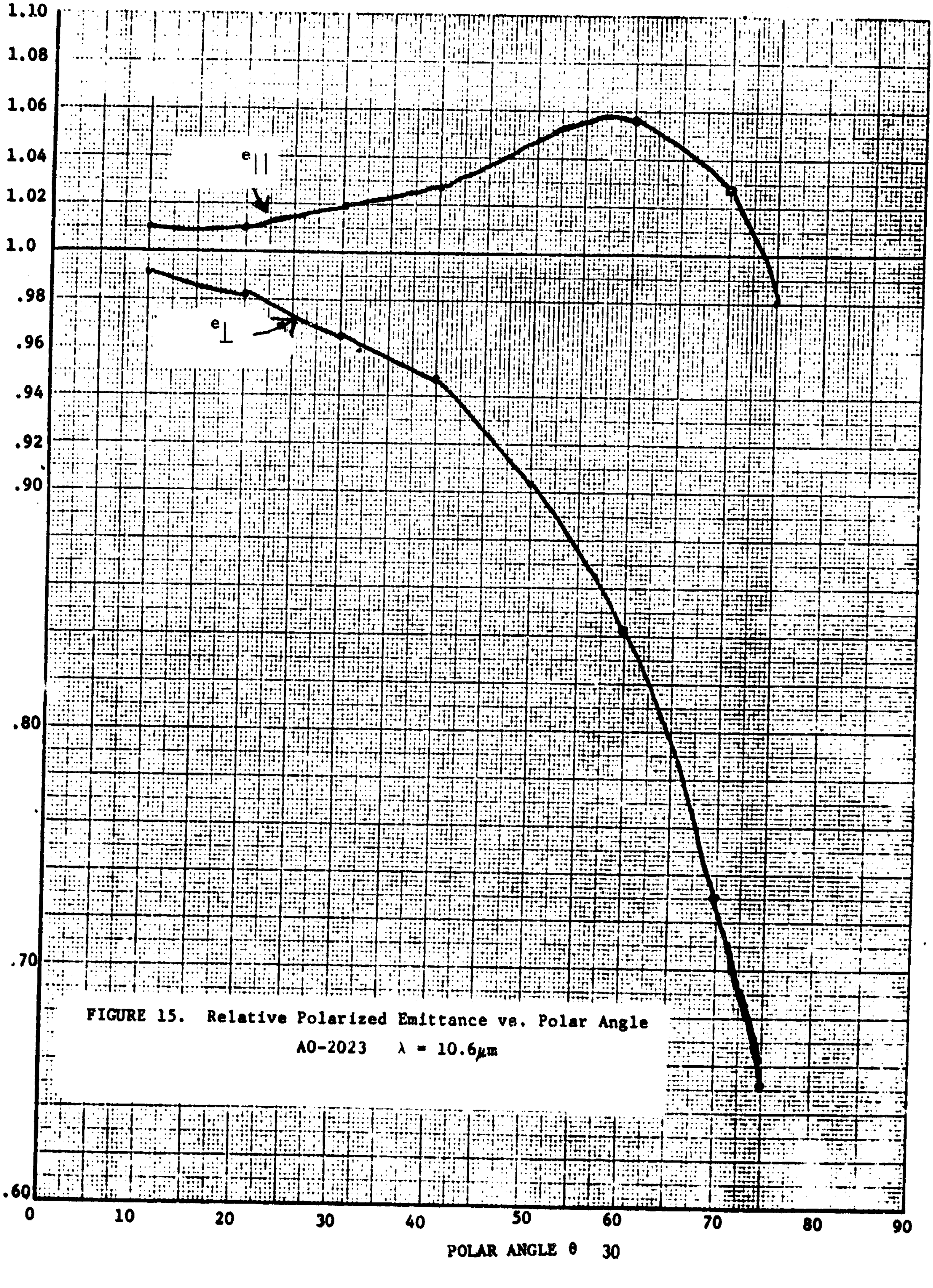


FIGURE 15. Relative Polarized Emittance vs. Polar Angle
AO-2023 λ = 10.6μm

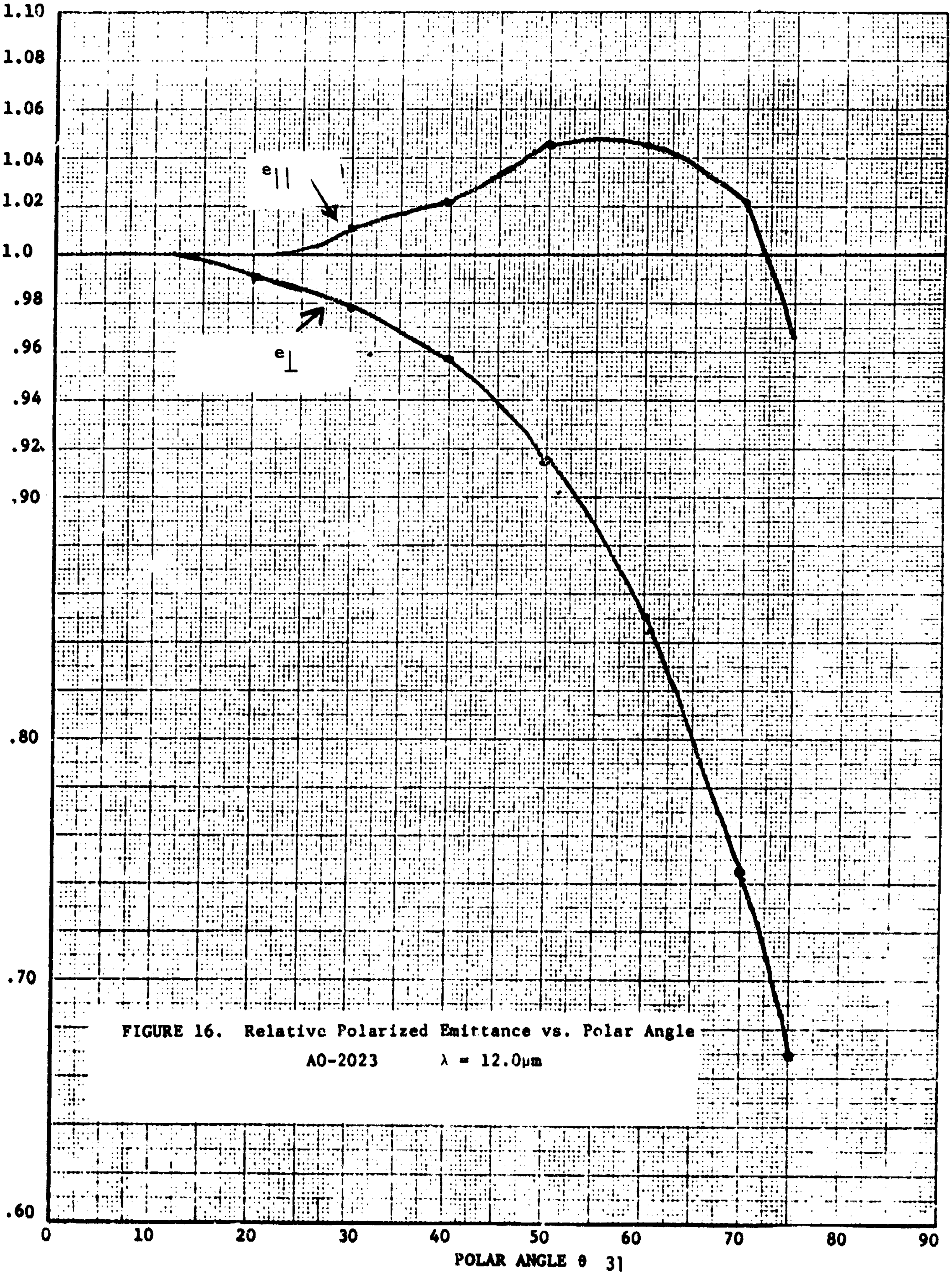


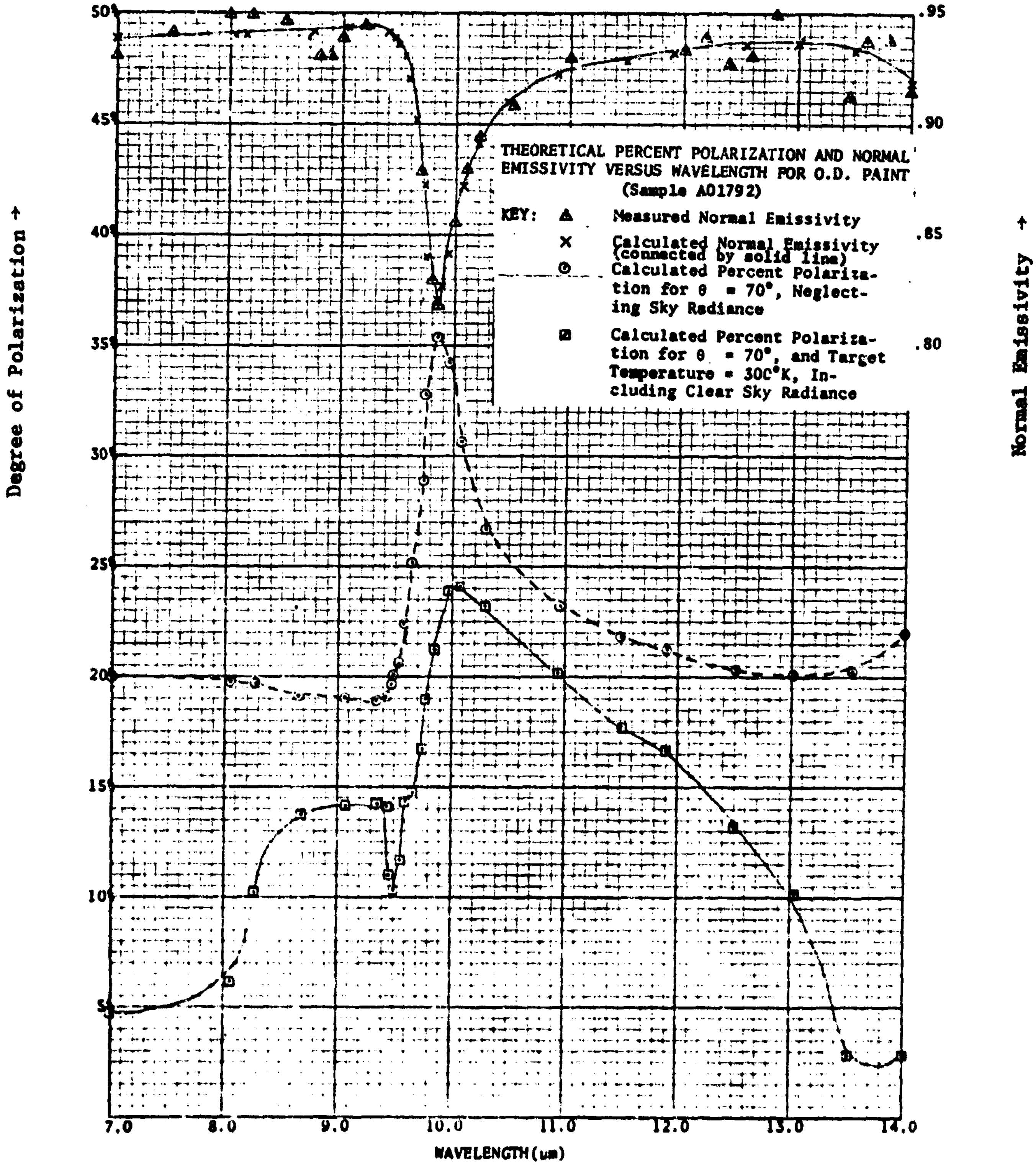
FIGURE 16. Relative Polarized Emittance vs. Polar Angle

A0-2023 λ = 12.0μm

4. MODEL VALIDATION

Figure 17 shows results of the emittance model for an O. D. paint, calculated last year as part of the Target Signature Analysis Program of ERIM, for the U. S. Air Force. In this figure the degree of polarization of the emittance of an O. D. paint sample was calculated as a function of wavelength for the case of no reflective input other than clear sky radiance. The target was assumed to be at a temperature $T = 300°K$ and the angle of observation was chosen to be $\theta_r = 70°$. In this theoretical treatment, the paint was assumed to be a perfectly specular surface, with neglible volume and multi-surface reflection. A normal-incidence reflectivity curve was fit with the classical oscillator model discussed above to find values for the complex index of refraction $N = n - ik$ as a function of wavelength. These indices were then fed into Fresnel equations for $R_{||}$ and $R_{\perp}$ (Eq. 3) from which $E_{||}(\theta)$ and $E_{\perp}(\theta)$ were calculated from Eq. (2). Emission polarization was then calculated from Eq. (1).

The degree of polarization of most naturally-occurring materials is low in the thermal IR, compared to the polarization of painted surfaces. The only known measurements of emission polarization from natural materials are given in Table I, which shows the degree of polarization for a few natural targets measured broadband (approximately 8 to 14μm) under clear, humid sky conditions [3]. The highest degree of polarization is approximately 2% for these materials, as compared with approximately 9% for an O.D. paint sample measured at the same angle ($\theta = 75°$) under the same conditions. Had the measurements been in a 2μm-wide band centered near 9.8μm, Figure 17 predicts that for the O.D. paint the degree of polarization would have been appreciably higher. The increase in the degree of polarization in the reststrahlen band for target materials may be useful in the discrimination of such targets from backgrounds like water, which also can have a high degree of polarization.



THEORETICAL PERCENT POLARIZATION AND NORMAL EMISSIVITY VERSUS WAVELENGTH FOR O.D. PAINT
(Sample A01792)
KEY:
Measured Normal Emissivity
Calculated Normal Emissivity (connected by solid line)
Calculated Percent Polarization for θ = 70°, Neglecting Sky Radiance
Calculated Percent Polarization for θ = 70°, and Target Temperature = 300°K, Including Clear Sky Radiance
Degree of Polarization →
Normal Emissivity →
50%
45%
40%
35%
30%
25%
20%
15%
10%
5%
.95
.90
.85
.80
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
WAVELENGTH (μm)

FIGURE 17

TABLE I

POLARIZATION FIELD MEASUREMENTS

(August 5, 1970, Clear Sky Conditions, Willow Run Airport)

Name	θ (Measured from average macroscopic surface normal)	$L_{\parallel}$ ($\frac{mw}{cm^2 sr}$)	$L_{\perp}$ ($\frac{mw}{cm^2 sr}$)	$\frac{L_{\parallel} - L_{\perp}}{L_{\parallel} + L_{\perp}}$
Packed Beach Sand	75°	4.80	4.63	.0180
Packed Beach Sand	60°	4.88	4.82	.0062
Wet Sand	75°	5.08	4.88	.0208
Granite Rock (Irregular shape, natural surface)	75°	5.37	5.16	.0199

$L_{\parallel}$ = detected radiance from target with electric vector vibrating parallel to plane of emission

$L_{\perp}$ = detected radiance from target with electric vector vibrating perpendicular to plane of emission

For the natural materials in Table I, the degree of polarization generally increased with increasing observation angle for $\theta > 50°$, but the measured polarization was so slight for $\theta < 50°$ that it fell below noise levels of the radiometer system. As for angular dependence of polarization from O. D. paint, Table II gives measured and calculated values for the degree of polarization of the emittance for θ from 10° to 70° for a wavelength of 9.83μm, the center of the reststrahlen band. For $\theta > 40°$ the emission polarization of paints can be quite large compared with that of natural target materials.

The good agreement between calculated results and the measured values shown in Table II were encouraging enough to justify further validation with respect to other O.D. paint samples. Under this BRL contract, three O.D. painted surfaces were studied using an ERIM spectrometer which enabled us to measure spectral radiance distributions as well as polarization dependent radiance as a function of observation angle. The samples are labeled 2017, 2022, and 2023.

Compared with the earlier sample (1792), these three O.D. paints exhibited less pronounced reststrahlen bands; hence, their degree of polarization is neither as large or as wavelength dependent. Table III shows the measured and calculated (from the above model) degree of polarization for the three O.D. paints 2017, 2022, and 2023 at angular increments of 10° for wavelengths of 10.6μm, 12.0μm, 9.7μm, 8.3μm, and 5.3μm. No calculations were made for the 5.3μm wavelength primarily because the data were very noisy below 7μm.

As can be observed from the "Model Result" and "Measured" columns, the model always predicts a higher degree of polarization than is measured, owing to the assumptions in the model that the paint surfaces are perfectly smooth and that the paint layer is optically thick. The middle column under each paint sample shows the product of multiplying the sample result times a constant factor of 0.75. The physical reason for choosing a constant

correction factor is that the surface roughness should affect radiation from all wavelengths and angles about the same, if the roughness is on a much different scale of magnitude than the wavelength variation (5μm - 12μm) used for the calculations of this model. The magnitude of the constant factor, however, was chosen solely on an empirical basis. As shown in Table III, the product of the model result and the 0.75 factor is within experimental error of the polarization measurements for 6 of 6 measurements on O. D. paint 2017, for 22 of 28 measurements on O.D. paint 2022, and for 15 of 27 measurements on O.D. paint 2023. The calculation of experimental error is explained in Appendix A. Overall, these calculated results for three paint samples and 4 wavelengths fell within experimental error for 43 of 61 measurements, or 70% of the time. On this basis, the model (including the 0.75 constant multiplicative factor) has been verified for degree of polarization calculations.

Figures 18, 19, and 20 are plots of relative polarized emittance versus polar angle at $\lambda = 10.6\mu m$ for O.D. paints 2017, 2022, and 2023 respectively. They show how the parallel and perpendicular components of emittance calculated by the model compared with experimental measurements. No multiplicative or other factors have been employed to alter the oscillator model results in these figures. The relative polarized emittances are

$e_{||}(\theta) = \frac{E_{||}(\theta)}{E(0)}$ and $e_{\perp}(\theta) = \frac{E_{\perp}(\theta)}{E(0)}$. Figure 18 shows a good correlation between theoretical and observed relative polarized emittances for paint 2017, where 4 unpolarized, near-normal spectral emittance curves were averaged to produce the input for the oscillator model. Figure 19 shows what can happen when the unpolarized spectral emittance curves have measurement discrepancies. An average of the best two curves was used as oscillator model input to produce the dashed line. The two worst curves were used to produce the results shown by the rectangles, and the circles show what happens when all four curves are averaged prior to application of the

TABLE II

COMPARISON OF THEORETICALLY CALCULATED AND EXPERIMENTALLY MEASURED DEGREE OF POLARIZATION FOR EMITTANCE FOR $\lambda = 9.83\mu m$ (O.D. Paint A01792)

θ	Calculated Degree of Polarization	Measured Degree of Polarization
10°	0.58%	0.25%
20°	2.37%	1.06%
30°	5.45%	3.47%
40°	10.03%	7.50%
50°	16.35%	12.56%
60°	24.71%	20.25%
70°	35.44%	32.46%

TABLE III

COMPARISON OF THEORETICALLY CALCULATED AND EXPERIMENTALLY

MEASURED DEGREE OF POLARIZATION FOR O.D. PAINTS

	θ_r	O.D. Paint A02017			O.D. Paint A02022			O.D. Paint A02023		
		Calculated (%)		Measured (%)	Calculated (%)		Measured (%)	Calculated (%)		Measured (%)
		Model Result	Multiplied by 0.75		Model Result	Multiplied by 0.75		Model Result	Multiplied by 0.75	
λ = 10.6μm	10°	0.3	0.2	0.3±1.9	0.3	0.2	0.3±1.5	0.6	0.5	0.9±1.8
	20°	1.4	1.0	1.9±1.9	1.3	1.0	1.0±1.5	2.3	1.7	1.4±1.8
	30°	3.3	2.5	2.8±1.9	2.1	2.3	2.2±1.5	5.1	3.8	2.7±1.8
	40°	6.1	4.6	4.5±1.9	5.7	4.3	4.3±1.5	9.0	6.8	4.1±1.8
	50°	10.2	7.7	7.7±1.9	9.5	7.1	7.0±1.5	13.7	10.3	7.3±1.8
	60°	15.9	11.9	12.3±2.0	14.6	11.0	11.4±1.6	19.2	14.4	11.3±1.9
	70°	23.7	17.8	-	21.4	16.1	16.7±1.7	25.5	19.1	17.0±2.1
λ = 12.0μm	10°				0.3	0.2	<0.3±1.9	0.4	0.3	<0.5±2.0
	20°				1.1	0.8	0.7±1.9	1.8	1.4	<0.5±2.0
	30°				2.6	2.0	2.6±1.9	4.1	3.1	1.6±2.0
	40°				5.0	3.8	4.5±1.9	7.5	5.6	3.3±2.0
	50°				8.4	6.3	7.5±1.9	12.0	9.0	6.6±2.0
	60°				13.3	10.0	12.0±2.0	17.6	13.2	10.2±2.1
	70°				20.0	15.0	18.0±2.2	24.7	18.5	15.7±2.3
λ = 9.7μm	10°				0.4	0.3	<0.3±2.0	0.7	0.5	<0.5±2.0
	20°				1.7	1.3	1.3±2.0	2.7	2.0	<0.5±2.0
	30°				3.8	2.9	2.9±2.0	5.9	4.4	2.4±2.0
	40°				6.9	5.2	5.4±2.0	10.0	7.5	4.6±2.0
	50°				11.0	8.3	9.7±2.0	14.7	11.0	8.0±2.0
	60°				16.2	12.2	14.6±2.1	19.8	14.9	12.3±2.1
	70°				22.6	17.2	21.7±2.4	25.3	19.0	18.6±2.4
λ = 8.3μm	10°				0.4	0.3	<0.3±1.8	0.8	0.6	1.0±1.9
	20°				1.8	1.4	0.7±1.8	3.3	2.5	1.6±1.9
	30°				4.2	3.2	2.0±1.8	7.1	5.3	3.5±1.9
	40°				7.4	5.6	3.5±1.8	11.5	8.6	5.6±1.9
	50°				11.3	8.5	6.3±1.8	15.9	11.9	9.8±1.9
	60°				15.4	11.6	9.5±1.9	20.0	15.0	15.6±2.0
	70°				19.6	14.7	15.0±2.1	23.8	17.9	-
λ = 5.3μm	10°						0.2			-
	20°						0.8			0.3
	30°						1.8			1.5
	40°						3.2			2.9
	50°						5.5			5.1
	60°						9.0			8.7
	70°						13.9			[illegible]

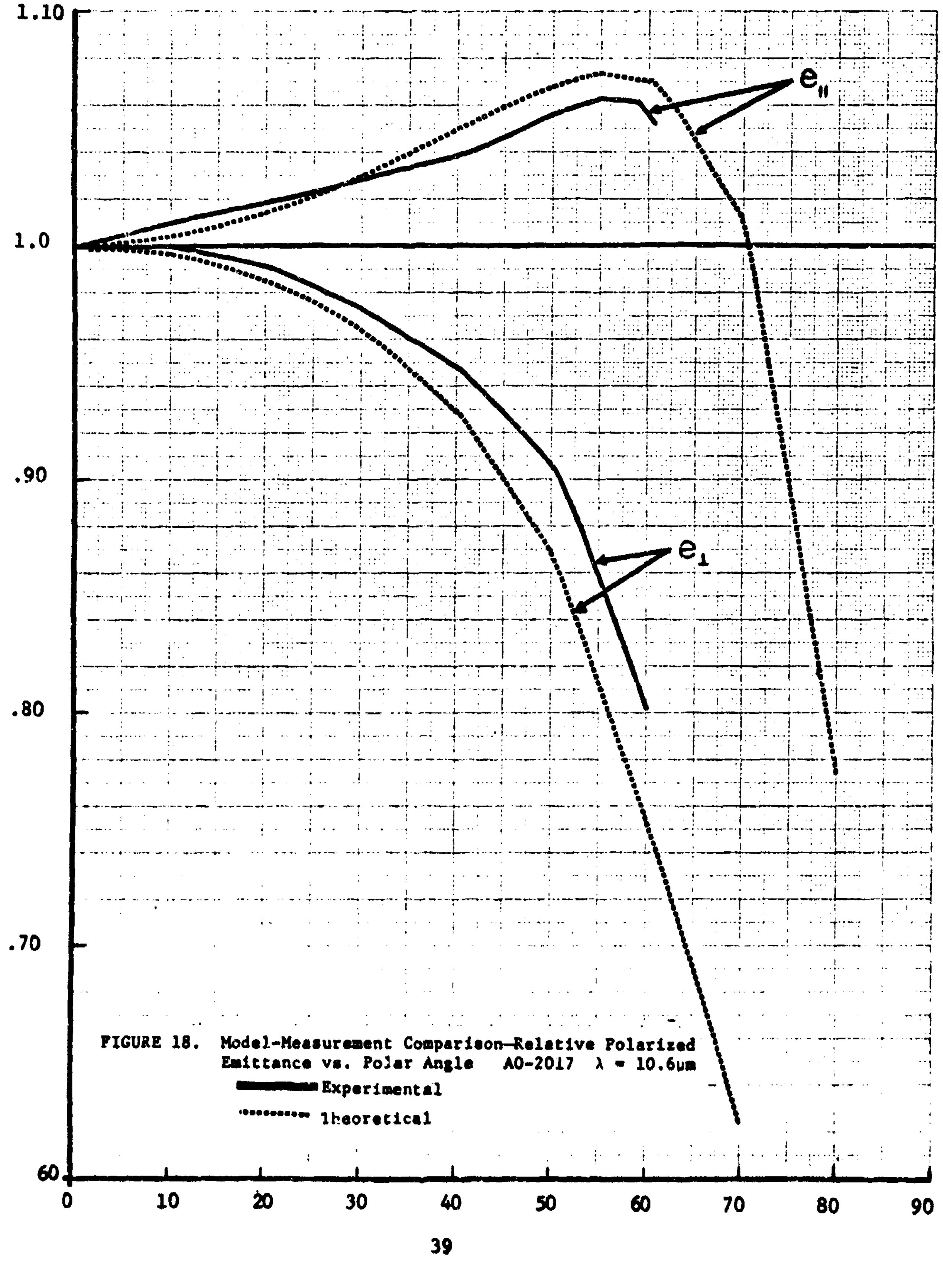


FIGURE 18. Model-Measurement Comparison—Relative Polarized Emittance vs. Polar Angle A0-2017 $\lambda = 10.6\mu m$

Experimental

Theoretical

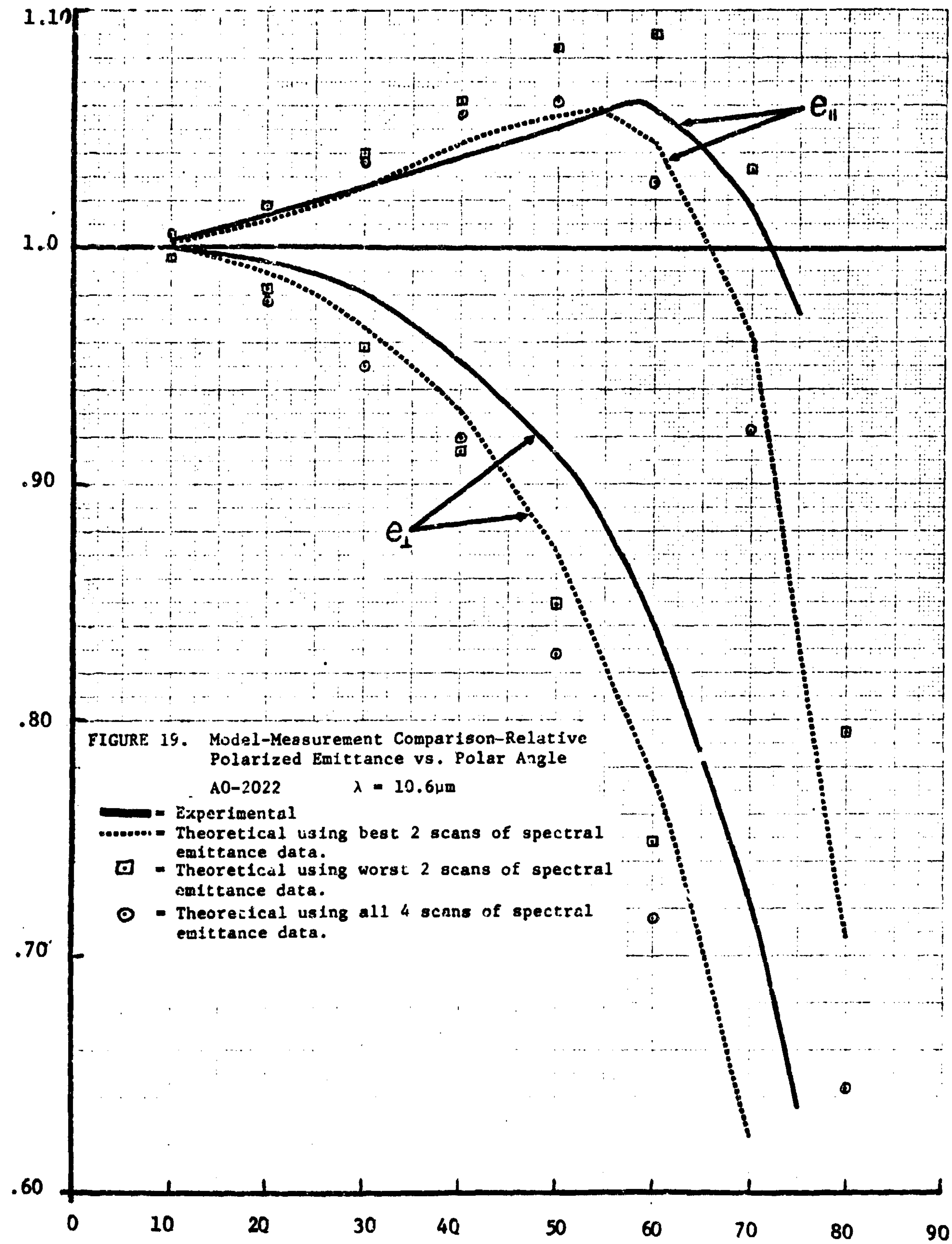


FIGURE 19. Model-Measurement Comparison-Relative Polarized Emittance vs. Polar Angle

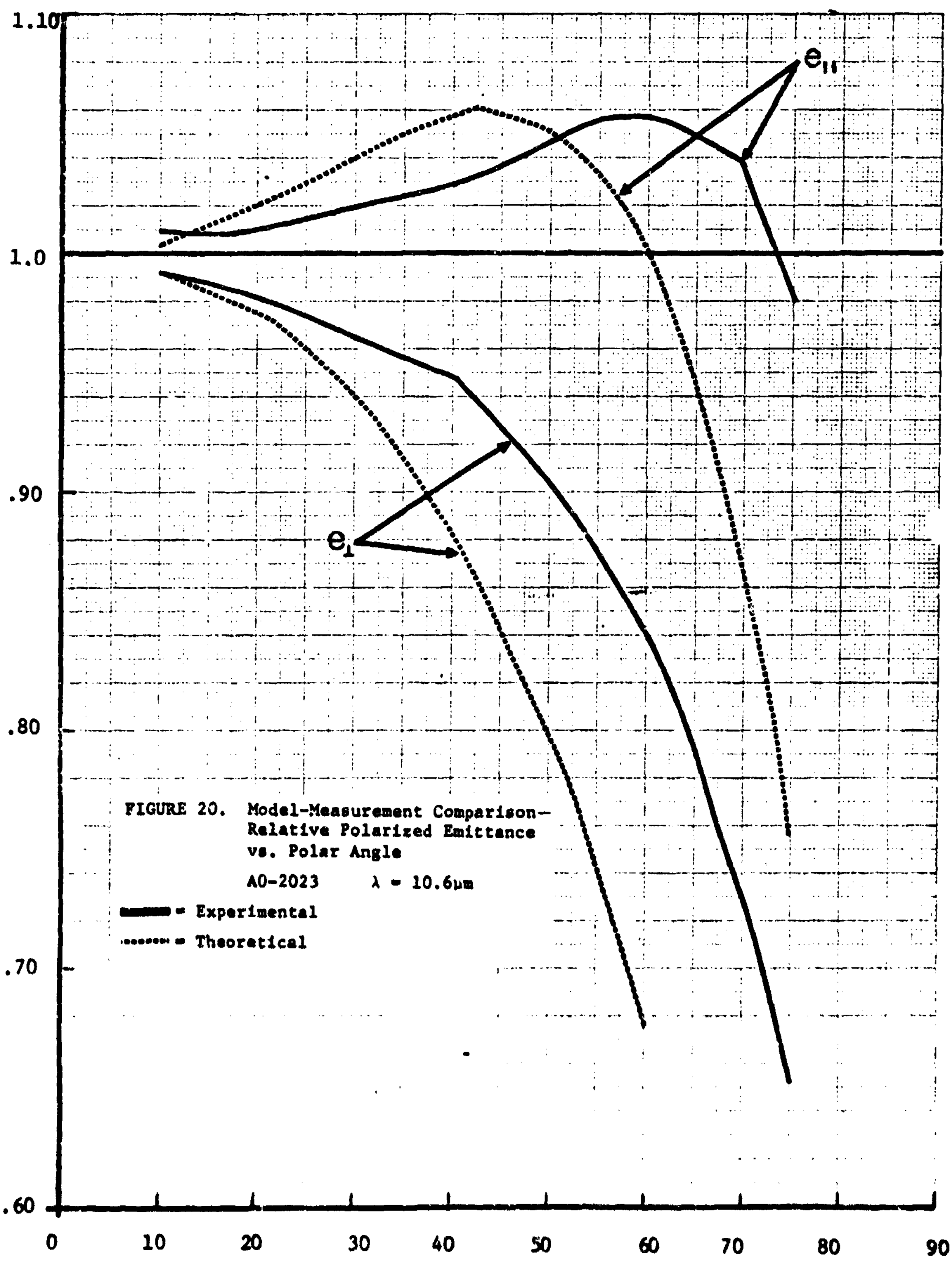


FIGURE 20. Model-Measurement Comparison—Relative Polarized Emittance vs. Polar Angle

A0-2023 $\lambda = 10.6\mu m$

▬▬ = Experimental

······ = Theoretical

oscillator model. This points out the need for better spectral emittance measurements as inputs to the model. Figure 20 shows the poorer results with paint 2023. The oscillator model was applied twice to the average of 4 spectral emittance curves, with almost the same results. The poorer agreement in Figure 20 is obvious also in the smaller than expected calculated degree of polarization results of Table III for paint 2023.

5. CONCLUSIONS

The oscillator model for calculating polarized components of spectral emittance and degree of polarization in the thermal infrared region for smooth-surfaced targets has produced theoretical values that are within experimental measurement accuracy 70% of the time. The accuracy of the model could be improved with better measurements of unpolarized, near-normal spectral emittance values. Such measurements could be improved by utilizing a parabolic reflectometer in the reflection mode instead of FISR, in the emission mode because of the greater absolute accuracy afforded by the former. FISR measurements would still probably be preferred for the relative polarized emittance versus polar angle measurements, because of the induced polarization inherent to the parabolic reflectometer. The model itself could probably be improved by accounting for thin-film transmission of paint on metal, but this might not be required after better spectral emittance measurements are available.

Although the O.D. paints used in this investigation are similar in spectral emittance features, the oscillator model should work at least as well for other smooth-surfaced materials which exhibit marked dispersion (high λ-dependence of the spectral emittance) in the thermal IR region, such as teflon, mylar, and possibly phenolics.

The most important feature of this model is that the degree of polarization can be calculated for smooth-surfaced materials in the thermal IR region for any λ (from about 7 to 15μm) and any polar angle, with only a measurement of spectral emittance from 7 - 15μm at near-normal incidence required. This will save considerable time and money on experimental measurements.

APPENDIX A

DETERMINATION OF EXPERIMENTAL ERROR IN MEASUREMENT OF DEGREE OF POLARIZATION

The equation for degree of polarization can be written as:

$$P_E(\theta) = \frac{E_{||}(\theta) - E_{\perp}(\theta)}{E_{||}(\theta) + E_{\perp}(\theta)} = \frac{e_{||}(\theta) - e_{\perp}(\theta)}{e_{||}(\theta) + e_{\perp}(\theta)} \qquad \text{(A-1)}$$

where $e_{||}(\theta) = \dfrac{E(\theta)_{||}}{E(0)}$ = relative polarized emittance, parallel component

$e_{\perp}(\theta) = \dfrac{E(\theta)_{\perp}}{E(0)}$ = relative polarized emittance, perpendicular component

All of the above and following parameters are wavelength and angle dependent, but the λ and θ notation will be suppressed here.

The error in P_E due to errors in measured values of $e_{||}$ and $e_{\perp}$, respectively, can be represented by:

$$\Delta P_{E||} = \left[\frac{1}{e_{||} + e_{\perp}} - \frac{e_{||} - e_{\perp}}{(e_{||} + e_{\perp})^2}\right] \Delta e_{||} = \frac{2e_{\perp}}{((e_{||} + e_{\perp})^2} \Delta e_{||} \qquad \text{(A-2)}$$

$$\Delta P_{E\perp} = \left[- \frac{1}{e_{||} + e_{\perp}} - \frac{e_{||} - e_{\perp}}{(e_{||} + e_{\perp})^2}\right] \Delta e_{\perp} = \frac{-2e_{||}}{(e_{||} + e_{\perp})^2} \Delta e_{\perp} \qquad \text{(A-3)}$$

The total error in P_e can be described as:

$$\Delta P_E = \sqrt{(\Delta P_{||})^2 + (\Delta P_{\perp})^2} = \left[\frac{2}{(e_{||} + e_{\perp})^2}\right] \sqrt{(e_{\perp}\,\Delta e_{||})^2 + (e_{||}\Delta e_{\perp})^2} \qquad \text{(A-4)}$$

Let σ_p be the precision error in the measurement of unpolarized spectral emittance. It will be assumed that $\Delta e_{||}$ and $\Delta e_{\perp}$ are equal and that the addition of a polarizer into the optical system increases the precision

error by a factor of $\sqrt{2}$, such that

$$\Delta e_{||} = \Delta e_{\perp} = \sqrt{2}\,\sigma_p \tag{A-5}$$

When equation (A-5) is substituted into equation (A-6), the resultant error in P_E from error measurements in $e_{||}$ and $e_{\perp}$ is:

$$\Delta P_E = \frac{2\sigma_p}{(e_{||} + e_{\perp})^2} \sqrt{2(e^2_{||} + e_{\perp}^2)} = 2.828\,\sigma_p \frac{\sqrt{e^2_{||} + e^2_{\perp}}}{(e_{||} + e_{\perp})^2} \tag{A-6}$$

The ΔP_E is multiplied by 100 in Table III to get % ΔP_E. It can be observed from equation (A-6) that ΔP_E is not a strong function of the values of $e_{||}$ and $e_{\perp}$, and that $\Delta P_E \approx 2.828\sigma_p$ for small θ, where $e_{||}$ and $e_{\perp}$ are near 1.0 in value.

APPENDIX B

DOCUMENTATION FOR CLASSICAL

OSCILLATOR FITTING PROGRAM

The oscillator fitting program is designed to compute oscillator parameters from which effective indices of refraction can be calculated, according to Eq. (1) of the text. Initial estimates of the number of oscillators responsible for spectral features of the specimen and the strengths (S), frequency positions (NU = $\frac{\lambda}{10,000}$, for λ in μm), and widths (GAMMA) of each oscillator must be made. The dielectric constant at infinite frequency (E) must also be made known. [Note: Here E = E_∞.]

To begin with one assumes at least one oscillator is located at each reflectance maximum in the infrared reflectance spectrum. This determines the initial number of oscillators and their positions (NU). The initial values of E, S, and GAMMA can be taken to be equal to the values determined for the O.D. paint 2017 in Table B-1. Table B-1 gives the result of the oscillator fitting program for the three O.D. paints listed in Table 1 of the text.

The program will refine the position, strength, and shape of the given oscillators, but it will not add or delete oscillators. However, if an oscillator is grossly superfluous, the strength will be decreased, and/or the width will be increased, to such an extent as to make its contribution negligible.

The program returns an error parameter before supplying the new oscillator parameters. If the error parameter is 0, convergence (under the input EPS and EST)* has taken place, otherwise it has not. Whether or not convergence has taken place, it is often advisable to look at the oscillator parameters and the emittance values calculated from them to decide if additional oscillators should be added and/or subtracted, or whether the limiting conditions (ESP, EST) should be changed. If the theoretical and experimental reflectance curves do not quantitatively match, i.e. do not peak and trough near the same wavelengths, addition or subtraction of an oscillator is called for. In general, two things are

*See last page of this Appendix for definitions.

necessary to judge a good fit: a sum of the differences squared (between theoretical and experimental spectral reflectance) less than about 10^{-2} and a qualitative match between peaks and valleys of experimental and theoretical spectral reflectance curves. For low-contrast materials (small reststrahlen bands), a good quantitative fit is usually not a sufficient criterion for successful fitting, as seen by the results for sample 2023 in Table B-1 and Table 1 of the text. (See discussion in text of Appendix C.)

TABLE B-1

EFFECTIVE OSCILLATOR PARAMETERS FOR POINTS RESULTING

FROM CLASSICAL OSCILLATOR FITTING PROGRAM

O. D. Paint Sample	Oscillator Parameters			
	E	S	NU	GAMMA
A02017	1.040	0.5421 0.1053	993.7 1373.9	0.3234 0.4264
A02022	1.051	0.0866 0.5716	787.8 988.4	0.1190 0.4168
A02023	.728	1.076 .2456	828.0 1022.6	.7384 4.683

DATA DECK FOR THE OSCILLATOR PROGRAM

CARD #	FORMAT	VARIABLES(s)	DESCRIPTION
1	20A4	A	Any title up to 80 characters in length (including blanks).
2	I5, E15.5, and F10.0	LIMIT,EPS,EST	LIMIT = number of interations desired (30 is a good choice); EPS = test value for the expected absolute error (see the write-up on FMFP; despite what it says 0.05 has worked reasonably well); EST = estimated value of F(x) (also see Appendix F).
3	I5	N	Three times the number of cards of type 4, plus 1 (i.e., total number of parameters needed to describe all the oscillators with card types 4 and 5).
4	3F10.0	S,NU,GAMMA	S = strength of the oscillator; NU = location of the oscillaotr (in wave numbers); GAMMA = width of oscillator.
5	F10.0	E	Dielectric constant at infinite frequency
6	I5	M	Number of points used to describe the curve (i.e., no. of cards of type 7).
7	2F10.0	WIN(I),RIN(I)	WIN(I) = wave number for the data point; RIN(I) = percent emittance at WIN(I). Use as many of these as necessary to throughly delineate the curve (at least 45-50).

APPENDIX C

DOCUMENTATION FOR PROGRAM 'EMISPOL'.

EMISPOL is a straightforward program, in which the oscillator parameters from the previous program are input parameters. Output is degree of polarization (PERPOL) and $e_{||}(\theta)$ and $e_{\perp}(\theta)$, relative emittance components.

Where reststrahlen bands are small, it is important to note that the index of refraction as determined by the oscillator program is not reliable. If band structure is not pronounced it is difficult to determine suitable oscillator parameters. On the other hand, the emissivity is then not very spectrally dependent, which means that it is reasonable to regard the refractive index as constant over the same wavelength region.

Under these circumstances it is valid to by-pass the oscillator program and feed a constant value for refractive index into EMISPOL. Doing so requires a slight modification of EMISPOL. Immediately after statement 600 (see EMISPOL listing in Appendix E), the program calls in a subroutine which calculates n and k given the final oscillator parameters. This subroutine (and hence the oscillator program) can be by-passed by substituting a statement which supplies values for n and k. Values can be determined from the Brewster angle as described in Volume I of this report.

DATA DECK FOR EMISPOL

CARD #	FORMAT	NAME	DESCRIPTION AND/OR COMMENTS
1	10A4	ITITLE	Any title information, up to 80 characters.
2	I3	K	No. of Lamdas (wavelengths) to be provided (a maximum of 185; see card 10).
3	F5.3	EPS	E from Program OSSC.
4	I2	NPTS	No. of Oscillators (a maximum of 8).
5	7F8.2	FR(I)	NU values from Program OSSC.
6	7F8.4	S(I)	S values from Program OSSC.
7	7F8.4	G(I)	GAM values from Program OSSC.
8	I3	M	No. of AI's (a maximum of 10) (see card 11).
9	I3	T	Temperature of the object which is emitting (in degrees K).
10	10F8.3	LAMDA(J)	Lamda's at which emittance polarization is calculated for each AI(N).
11	F10.6	AI(N)	Angles of incidence (1 per card).

APPENDIX D

PROGRAM LISTING - OSCILLATOR

```
      DIMENSION RFD(13,600),D1(602),D2(602)
      DIMENSION WIN(300),RIN(300)
      DIMENSION LABEL(6)
      DIMENSION LBK(9),LBL(9),LBM(2)
      REAL XS(25),H(27)
      REAL X(25),G(25),B(1000),A(20),DATA(250)
      DATA LBL/36H                ALPHA              /
      DATA LABEL/4H  R ,4H E1 ,4H,E2 ,4H-EF ,4H  N ,4H  K  /
C     ***********************************************************
      READ(5,548)A,LIMIT,EPS,EST
  548 FORMAT(20A4,/I5,E15.5,F10.0)
C     ***********************************************************
      READ(5,55)N
   55 FORMAT(I5)
C     ***********************************************************
      READ(5,5)(X(I),I=1,N)
5     FORMAT(3F10.0)
C     -----------------------------------------------------------
      WRITE(6,40)A,LIMIT,EPS,EST
40    FORMAT(1H1,20A4,/' LIMIT OF ITERATIONS IS',I5,'  EPS IS ',E15.5,//
     .' ESTIMATED F(X)= ', F12.5,/)
C     -----------------------------------------------------------
      WRITE(6,470)
  470 FORMAT(5X,'INITIAL GUESSES FOR OSCILLATOR PARAMETERS ARE  '// )
      NM=N-1
C     -----------------------------------------------------------
      WRITE(6,471) (X(I),I=1,NM)
471   FORMAT(14X,'S',16X,'NU',14X,'GAMMA',//(5X,E12.5,8X,E12.5,
     . 8X,E12.5))
C     -----------------------------------------------------------
      WRITE(6,472)X(N)
  472 FORMAT(3X,   'E(INF)= ' ,F12.4)
C     ***********************************************************
      READ(5,55)   M
C     -----------------------------------------------------------
      WRITE(6,1766)M
 1766 FORMAT('   CARD COUNT IS  ' ,I5)
C     -----------------------------------------------------------
      WRITE(6,2000)
 2000 FORMAT('1REFLECTIVITY BASED ON INITIAL GUESSES'/)
C     -----------------------------------------------------------
      WRITE(6,487)
C     ***********************************************************
      READ(5,555)(WIN(I),RIN(I),I=1,M)
  555 FORMAT(2F10.0)
      DO 29  I=1,N
29    X(I)=SQRT(X(I))
      ZTL=0
      DO 10  J=1,M
      RIN(J)=RIN(J)/100.
      YY=FUNX(N,X,WIN(J))
      Z=YY-RIN(J)
      ZLT=ZLT+Z*Z
C     -----------------------------------------------------------
      WRITE(6,16) WIN(J),RIN(J),YY,Z
   10 CONTINUE
C     -----------------------------------------------------------
      WRITE(6,1112)ZLT
 1112 FORMAT( 5X,' SUM OF THE DIFFERENCES SQUARED IS  ',E12.4)
      CALL FUNCTI(M,WIN,RIN)
```

```
      EXTERNAL FUNCT
      IF(LIMIT .EQ. 0)GO TO 250
      CALL FMFP(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,B)
  250 CONTINUE
      DO 19  I=1,N
19    XS(I)=X(I)**2
C     ------------------------------------------------------------
      WRITE(6,9745)
 9745 FORMAT(1H1)
C     ------------------------------------------------------------
      WRITE(6,473)F,IER
  473 FORMAT(3X,///'FITTING HAS BEEN COMPLETED WITH F(X)=  ',E15.8,//
     .'  AND ERROR PARAMETER =  ',I5//'  FITTED VALUES FOR OSCILLATOR',
     .' PARAMETERS ARE  '/)
C     ------------------------------------------------------------
      WRITE(6,471)(XS(I),I=1,NM)
      WRITE(6,472)XS(N)
      WRITE(6,487)
  487 FORMAT(1H1,3X'ENERGY       R(EXP)      R(FITTED)   DIFFERENCE'/ )
      ZLT=0
      DO 13 J=1,M
      YY=FUNX(N,X,WIN(J))
      Z=YY-RIN(J)
      ZLT=ZLT+Z*Z
C     ------------------------------------------------------------
      WRITE(6,16)WIN(J),RIN(J),YY,Z
   16 FORMAT(1X,4F12.5)
13    CONTINUE
C     ------------------------------------------------------------
      WRITE(6,1112)ZLT
      END


      SUBROUTINE FUNCTI(M,WIN,RIN)
      DIMENSION WIN(300),RIN(300)
      RETURN
      ENTRY FUNCT(N,X,VAL,GRAD)
      REAL X(25),GRAD(25)
      REAL W(10),S(10),G(10)
      REAL P(300),Q(300),V(300)
      COMPLEX Z,D(300,10),E(300),H(300)
      NN=N/3
      DO 1 I=1,NN
      L=3*(I-1)
      S(I)=X(L+1)
      W(I)=X(L+2)
    1 G(I)=X(L+3)
      EINF=X(N)
      DO 2 J=1,NN
      W2=1./W(J)**2
      G2=G(J)**2
      DO 2 I=1,M
      WW=WIN(I)*W2
    2 D(I,J)=S(J)/CMPLX(1.-WW**2,-WW*G2)
      DO 3 I=1,M
      E(I)=EINF**2
      DO 4  J=1,NN
```

```
    4 E(I)=E(I)+S(J)*D(I,J)
      E(I)=CEXP(.5*CLOG(E(I)))
      IF(REAL(E(I)).LT.C.)E(I)=-E(I)
      P(I)=CABS(E(I))**2-2.*REAL(E(I))+1.
      Q(I)=P(I)+4.*REAL(E(I))
    3 V(I)=P(I)/Q(I)-RIN(I)
      VAL=0
      DO 33 I=1,M
   33 VAL=VAL+V(I)**2
C     ----------------------------------------------------------------
      WRITE(6,76) VAL
   76 FORMAT(1X,E14.5)
      DO 7  I=1,M
      Z=CONJG(E(I))
    7 H(I)=8.*V(I)*.5*(Q(I)*(Z-1.)-P(I)*(Z+1.))/E(I)/Q(I)**2
      DO 6 J=1,NN
      L=3*(J-1)
      GRAD(L+1)=0
      GRAD(L+2)=0
      GRAD(L+3)=0
      W2=G(J)/W(J)**2
      W3=-G(J)**2/W(J)**3
      W5=-2./W(J)**5
      DO 6 I=1,M
      GRAD(L+1)=GRAD(L+1)+REAL(H(I)*D(I,J))
      Z=H(I)*D(I,J)**2*WIN(I)
      GRAD(L+2)=GRAD(L+2)+REAL(Z*CMPLX(WIN(I)*W5,W3)   )
      GRAD(L+3)=GRAD(L+3)-AIMAG(Z)*W2
6     CONTINUE
      GRAD(N)=0
      DO 8 I=1,M
    8 GRAD(N)=GRAD(N)+REAL(H(I))*EINF
      RETURN
      END



      FUNCTION FUNX(N,X,WIN)
      REAL X(25)
      REAL W(10),G(10),S(10)
      NN=N/3
      DO 1 I=1,NN
      L=3*(I-1)
      S(I)=X(L+1)
      W(I)=X(L+2)
      G(I)=X(L+3)
1     CONTINUE
      COMPLEX E
      E=X(N)**2
      DO  2 J=1,NN
      E=E+S(J)**2/CMPLX(1.-(WIN/W(J)**2)**2,-WIN*G(J)**2/W(J)**2)
2     CONTINUE
      E=CEXP(.5*CLOG(E))
      IF(REAL(E).LT.0.)E=-E
      FUNX=CABS((E-1.)/(E+1.))**2
      RETURN
      END
```

APPENDIX E

PROGRAM LISTING - EMISPOL

```
      DIMENSION LAMDA(185),AN(185),AK(185),AI(10),ER(185),EL(185)
      DIMENSION DE(185),NR(185),NL(185),DN(185),ITITLE(10),NSKY(9,185)
      DIMENSION FR(8),S(8),G(8),EE(185)
      DIMENSION PERPOL(185)
      COMMON FR,S,G
      COMMON NPTS,EPS
      REAL LAMDA,NSKY,NTAR,NR,NL
      INTEGER T
      INTEGER SKY
C     INPUT
100   READ (5,5) ITITLE
    5 FORMAT(10A4)
      WRITE (6,6) ITITLE
    6 FORMAT (1H1,10A4)
      READ (5,10) K
   10 FORMAT (I3)
      READ (5,12) EPS
   12 FORMAT (F5.3)
      READ (5,21) NPTS
   21 FORMAT (I2)
      READ (5,20) (FR(I),I=1,NPTS)
   20 FORMAT (8F8.2)
      READ (5,25) (S(I),I=1,NPTS)
   25 FORMAT (8F8.4)
      READ (5,25) (G(I),I=1,NPTS)
      READ (5,40) M
   40 FORMAT (I3)
   56 READ (5,60) T
   60 FORMAT (I3)
  609 READ (5,610) (LAMDA(I),I=1,K)
  610 FORMAT (10F8.0)
      N=0
  645 N=N+1
      READ (5,650) AI(N)
  650 FORMAT (F10.6)
      AI(N)=90.0-AI(N)
      DO 660 I=1,K
      NSKY(N,I)=0.0
      IF (N.GE.M) GO TO 600
      GO TO 645
  660 CONTINUE
C     CALCULATIONS
  600 DO 700 JJ=1,K
      CALL ANAK(LAMDA(JJ),AN(JJ),AK(JJ))
  700 CONTINUE
      DO 200 II=1,M
      AI(II)=AI(II)*3.1416/180.
      DO 150 JJ=1,K
      Q=SQRT(4.*(AN(JJ)**2)*(AK(JJ)**2)+((AN(JJ)**2)-(AK(JJ)**2)-SIN(AI(
     1II))**2)**2)
      A=0.5*(+AN(JJ)**2-AK(JJ)**2-(SIN(AI(II)))**2+Q)
      B=0.5*(-AN(JJ)**2+AK(JJ)**2+(SIN(AI(II)))**2+Q)
      RR=((SQRT(A)-COS(AI(II)))**2+B)/
     1   ((SQRT(A)+COS(AI(II)))**2+B)
      RL=(RR*((SQRT(A)-SIN(AI(II))*TAN(AI(II)))**2+B))/
     1        ((SQRT(A)+SIN(AI(II))*TAN(AI(II)))**2+B)
      NTAR=1.19E4/((LAMDA(JJ)**5)*((EXP(1.4388E4/(LAMDA(JJ)*T)))-1.0))
      ER(JJ)=1.0-RR
      EL(JJ)=1.0-RL
      EE(JJ)=.5*(ER(JJ)+EL(JJ))
```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```
      DE(JJ)=EL(JJ)-ER(JJ)
      NR(JJ)=(RR*NSKY(II,JJ)/2.0)+(ER(JJ)*NTAR/2.0)
      NL(JJ)=(RL*NSKY(II,JJ)/2.0)+(EL(JJ)*NTAR/2.0)
      DN(JJ)=NL(JJ)-NR(JJ)
      PERPOL(JJ)=(EL(JJ)-ER(JJ))/(EL(JJ)+ER(JJ))
  150 CONTINUE
      AI(II)=AI(II)*180./3.1416
      WRITE (6,70) AI(II),T,(LAMDA(L),AN(L),AK(L),NSKY(II,L),ER(L),EL(L)
     1,DE(L),NR(L),NL(L),DN(L),EE(L),PERPOL(L),L=1,K)
   70 FORMAT (//'AI= ',F8.3/,'TEMP= ',I5,/,1X,'LAMDA',3X,'AN',6X,'AK',6X
     1,'NSKY',7X,'ER',9X,'EL',9X,'DE',9X,'NR',9X,'NL',9X,'DN',9X,'EE',7X
     2,'PERPCL'/,(F6.2,2X,F6.4,2X,F6.4,2X,E10.4,1X,E10.4,1X,E10.4,1X
     3,E10.4,1X,E9.3,1X,E9.3,1X,E9.3,1X,E10.4,1X,E10.4))
  200 CONTINUE
      GO TO 100
      END




      SUBROUTINE ANAK(LAMBDA,AN,AK)
      DIMENSION FR(8),S(8),G(8)
      COMMON FR,S,G
      COMMON NPTS,EPS
      REAL LAMBDA
      F=10000./LAMBDA
      AE=0.
      BB=0.
      DO 110 KK=1,NPTS
      QQ=(S(KK)*((FR(KK))**2))/(((FR(KK))**2-F**2)**2+(G(KK)*FR(KK)*F)**
     12)
      AE=QQ*((FR(KK))**2-F**2)+AE
      BB=(.5*G(KK)*FR(KK)*F*QQ)+BB
  110 CONTINUE
      AA=AE+EPS
      AN=SQRT(.5*(AA+SQRT(AA**2+4.*(BB**2))))
      AK=BB/AN
      RETURN
      END
```

APPENDIX F

PROGRAM LISTING AND INSTRUCTIONS FOR IBM SCIENTIFIC SUBROUTINE - FMFP

(This material in this Appendix is a direct copy cf an IBM Scientific Subroutine as it appears in IBM Manual GH20-0205-4 of System/360 Scientific Subroutine Package, Version III, Programmer's Manual.)

Extremum of Functions

Subroutines FMFP and DFMFP

These subroutines perform the calculation of an unconstrained minimum of a function of several variables using a method proposed by Davidson. The underlying method is described in the article by R. Fletcher and M.J.D. Powell, "A Rapidly Convergent Descent Method for Minimization", Computer Journal, vol. 6, iss. 2, 1963, pp. 163 - 168.

It is assumed that the function f of the n variables $x_1, \ldots, x_n$ (abbreviated as argument vector x) may be computed together with its gradient vector g(x) for any point x. The generalized Taylor expansion for functions of several variables is

$$f(x+u) = f(x) + g(x) \cdot u + \frac{1}{2} u^T G(x) u + \text{higher terms}$$

where g is the gradient vector and G the matrix of second order partial derivatives. Vectors are assumed to be column vectors; u^T means transpose of vector u. It is assumed that in the neighborhood of the required minimum x_{min} the function is approximated closely by the first three terms of its Taylor expansion, giving

$$f(x) = f(x_{min}) + \frac{1}{2} (x - x_{min})^T G(x_{min}) (x - x_{min})$$

since $g(x_{min}) = 0$. Then the gradient is seen to be approximately $g(x) = G(x_{min}) (x - x_{min})$.

Assume now that the symmetric matrix G is positive definite. Then the following equation holds true:

$$x - x_{min} = G^{-1} (x_{min}) \cdot g(x)$$

which would allow x_{min} to be calculated in one step if $G^{-1} (x_{min})$ were available.

To approach $G^{-1} (x_{min})$, a method of successive linear searches in G-conjugate directions is used. Starting with the identity matrix $G^{(0)} = I$, a sequence of symmetric matrices $G^{(i)}$ is generated which tends to G^{-1}. At the $(i+1)^{st}$ iteration step a linear search is made in direction $h^{(i)} = - G^{(i)} g^{(i)}$, where $g^{(i)}$ is an abbreviation for $g(x^{(i)})$. By means of the linear search the minimum of $y(t) = f(x^{(i)} + t \cdot h^{(i)})$ is determined, giving argument $x^{(i+1)} = x^{(i)} + t_i \cdot h^{(i)}$.

The argument of the minimum $x^{(i+1)}$ on the line through $x^{(i)}$ in direction $h^{(i)}$ is determined by the relation that scalar product $(g^{(i+1)}, h^{(i)}) = 0$.

Now: $$x^{(n)} = x^{(j)} + \sum_{i=j}^{n-1} t_i h^{(i)}$$

and: $$g^{(n)} = g^{(j)} + \sum_{i=j}^{n-1} t_i \cdot Gh^{(i)}$$

Therefore:

$$\text{scalar product} \quad (g^{(n)}, h^{(j)}) = \sum_{i=j+1}^{n-1} t_i (Gh^{(i)}, h^{(j)})$$

Suppose now that the vectors $h^{(0)}, h^{(1)}, \ldots, h^{(n-1)}$ are G-conjugate, satisfying $(Gh^{(i)}, h^{(j)}) = 0$ for $i \neq j$. Then $(g^{(n)}, h^{(j)}) = 0$, and since $h^{(0)}, h^{(1)}, \ldots, h^{(n-1)}$ form a basis, $g^{(n)} = 0$ and $x^{(n)} = x_{min}$. This shows that the minimum is located at the n^{th} iteration for a quadratic function when using successive linear searches for G-conjugate directions.

For the generation of G-conjugate directions, start with $h^{(0)} = -g^{(0)}$ and calculate successive directions $h^{(i)}$ by means of $h^{(i)} = -G^{(i)}g^{(i)}$, where $G^{(i)}$ is modified to $G^{(i+1)}$ so that $h^{(i)}$ is an eigenvector of the matrix $G^{(i+1)}G$ with eigenvalue 1. This ensures that $G^{(i)}$ approaches G^{-1} as $x^{(i)}$ approaches x_{min}. An easy calculation shows:

$$G^{(i+1)} = G^{(i)} + \frac{dx \cdot dx^T}{dx^T \cdot dg} - \frac{G^{(i)}dg \cdot dg^T G^{(i)}}{dg^T G^{(i)} dg}$$

with $dg = g^{(i+1)} - g^{(i)}$

$dx = x^{(i+1)} - x^{(i)}$

where all vectors are regarded as column vectors, and superscript T means transpose of column vector--that is, row vector.

The strategy adopted for termination of the successive linear searches is as follows:

1. If the function value has not decreased in the last iteration step, the search for the minimum is terminated provided the gradient is already sufficiently small; otherwise, the next step is in the direction of steepest descent.

2. If the argument vector and the direction vec- change by very small amounts, and at least n iterations are performed, the minimization is terminated again.

3. If the number of iterations exceeds an upper bound furnished by the user, further calculation is bypassed, and an error code is set to 1 indicating poor convergence.

4. If one of the successive linear searches indicates that no constrained minimum exists, further calculation is bypassed again, and the error code is set to 2 indicating that it is likely that no minimum exists.
The i^{th} term $G^{(i)}$ is reset to the identity matrix if there is indication that the current $G^{(i)}$ is not positive definite, or if the formula for $G^{(i+1)}$ breaks down due to zero divisors.

The linear search technique used in subroutines FMFP and DFMFP is as follows. For a given argument vector x and a vector h defining a direction through x, a local minimum of the function $y(t) = f(x+th)$ is determined. This means that a value t_m must be determined such that $y'(t_m) = 0$.

Given $y'(t)$ = scalar product $(g(x+th), h)$, therefore $y(t)$ and $y'(t)$ may be calculated for any value of t, and:

$$y(0) = f(x) \text{ and } y'(0) = (g(x), h)$$

In case $y'(s2) = 0$, t_m is set equal to s2 and $x_m = x + s2$, h is used as argument of a constrained minimum on the line through x with direction h. In the second and third case a minimum lies between the points $x1 = x + s1 \cdot h$ and $x2 = x + s2 \cdot h$; that is, t_m must be in the interval (s1, s2).

The argument of the minimum is obtained by means of cubic interpolation using the function and derivative values at the points x1, x2. Let $x_3 = x + s3 \cdot h$ be the argument of the minimum of the third degree interpolation polynomial. Then:

$$s_3 = s2 - \alpha(s2 - s1) = s1 + (\alpha - 1)(s1 - s2)$$

with: $$\alpha = \frac{y'(s2) + w - z}{y(s2) - y'(s1) + 2w}$$

and: $$z = 3\,\frac{y(s2) - y(s1)}{s2 - s1} + y'(s1) + y'(s2)$$

$$w = \sqrt{[z^2 - y'(s1) \cdot y'(s2)]}$$

If $f(x3) \leqq f(x1)$ and $f(x3) \leqq f(x2)$, xm is set equal to x3 and used as argument of the wanted minimum along the given line. Otherwise the interval (x1, x2) is reduced by replacing x1 by x3 if $f(x3) \leqq f(x1)$ and $(g(x1), h) < 0$, and by replacing x2 by x3 in all other cases. Then the interpolation process is repeated for this new reduced interval.

```
C                                                                       FMFP  10
C     ..................................................................FMFP  20
C                                                                       FMFP  30
C        SUBROUTINE FMFP                                                FMFP  40
C                                                                       FMFP  50
C        PURPOSE                                                        FMFP  60
C           TO FIND A LOCAL MINIMUM OF A FUNCTION OF SEVERAL VARIABLES  FMFP  70
C           BY THE METHOD OF FLETCHER AND POWELL                        FMFP  80
C                                                                       FMFP  90
C        USAGE                                                          FMFP 100
C           CALL FMFP(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)                FMFP 110
C                                                                       FMFP 120
C        DESCRIPTION OF PARAMETERS                                      FMFP 130
C           FUNCT  - USER-WRITTEN SUBROUTINE CONCERNING THE FUNCTION TO FMFP 140
C                    BE MINIMIZED. IT MUST BE OF THE FORM               FMFP 150
C                    SUBROUTINE FUNCT(N,ARG,VAL,GRAD)                   FMFP 160
C                    AND MUST SERVE THE FOLLOWING PURPOSE               FMFP 170
C                    FOR EACH N-DIMENSIONAL ARGUMENT VECTOR  ARG,       FMFP 180
C                    FUNCTION VALUE AND GRADIENT VECTOR MUST BE COMPUTEDFMFP 190
C                    AND, ON RETURN, STORED IN VAL AND GRAD RESPECTIVELYFMFP 200
C           N      - NUMBER OF VARIABLES                                FMFP 210
C           X      - VECTOR OF DIMENSION N CONTAINING THE INITIAL       FMFP 220
C                    ARGUMENT WHERE THE ITERATION STARTS. ON RETURN,    FMFP 230
C                    X HOLDS THE ARGUMENT CORRESPONDING TO THE          FMFP 240
C                    COMPUTED MINIMUM FUNCTION VALUE                    FMFP 250
C           F      - SINGLE VARIABLE CONTAINING THE MINIMUM FUNCTION    FMFP 260
C                    VALUE ON RETURN, I.E. F=F(X).                      FMFP 270
C           G      - VECTOR OF DIMENSION N CONTAINING THE GRADIENT      FMFP 280
C                    VECTOR CORRESPONDING TO THE MINIMUM ON RETURN,     FMFP 290
C                    I.E. G=G(X).                                       FMFP 300
C           EST    - IS AN ESTIMATE OF THE MINIMUM FUNCTION VALUE.      FMFP 310
C           EPS    - TESTVALUE REPRESENTING THE EXPECTED ABSOLUTE ERROR.FMFP 320
C                    A REASONABLE CHOICE IS 10**(-6), I.E.              FMFP 330
C                    SOMEWHAT GREATER THAN 10**(-D), WHERE D IS THE     FMFP 340
C                    NUMBER OF SIGNIFICANT DIGITS IN FLOATING POINT     FMFP 350
C                    REPRESENTATION.                                    FMFP 360
C           LIMIT  - MAXIMUM NUMBER OF ITERATIONS.                      FMFP 370
C           IER    - ERROR PARAMETER                                    FMFP 380
C                    IER = 0 MEANS CONVERGENCE WAS OBTAINED             FMFP 390
C                    IER = 1 MEANS NO CONVERGENCE IN LIMIT ITERATIONS   FMFP 400
C                    IER =-1 MEANS ERRORS IN GRADIENT CALCULATION       FMFP 410
C                    IER = 2 MEANS LINEAR SEARCH TECHNIQUE INDICATES    FMFP 420
C                    IT IS LIKELY THAT THERE EXISTS NO MINIMUM.         FMFP 430
C           H      - WORKING STORAGE OF DIMENSION N*(N+7)/2.            FMFP 440
C                                                                       FMFP 450
C        REMARKS                                                        FMFP 460
C            I) THE SUBROUTINE NAME REPLACING THE DUMMY ARGUMENT  FUNCT FMFP 470
C               MUST BE DECLARED AS EXTERNAL IN THE CALLING PROGRAM.    FMFP 480
C           II) IER IS SET TO 2 IF , STEPPING IN ONE OF THE COMPUTED    FMFP 490
C               DIRECTIONS, THE FUNCTION WILL NEVER INCREASE WITHIN     FMFP 500
C               A TOLERABLE RANGE OF ARGUMENT.                          FMFP 510
C               IER = 2 MAY OCCUR ALSO IF THE INTERVAL WHERE F          FMFP 520
C               INCREASES IS SMALL AND THE INITIAL ARGUMENT WAS         FMFP 530
C               RELATIVELY FAR AWAY FROM THE MINIMUM SUCH THAT THE      FMFP 540
C               MINIMUM WAS OVERLEAPED. THIS IS DUE TO THE SEARCH       FMFP 550
C               TECHNIQUE WHICH DOUBLES THE STEPSIZE UNTIL A POINT      FMFP 560
C               IS FOUND WHERE THE FUNCTION INCREASES.                  FMFP 570
C                                                                       FMFP 580
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                  FMFP 590
C           FUNCT                                                       FMFP 600
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C                                                                       FMFP 610
C        METHOD                                                         FMFP 620
C           THE METHOD IS DESCRIBED IN THE FOLLOWING ARTICLE            FMFP 630
C           R. FLETCHER AND M.J.D. POWELL, A RAPID DESCENT METHOD FOR   FMFP 640
C           MINIMIZATION,                                               FMFP 650
C           COMPUTER JOURNAL VOL.6, ISS. 2, 1963, PP.163-168.           FMFP 660
C                                                                       FMFP 670
C     ..................................................................FMFP 680
C                                                                       FMFP 690
      SUBROUTINE FMFP(FUNCT,N,X,F,G,EST,EPS,LIMIT,IER,H)                FMFP 700
C                                                                       FMFP 710
C        DIMENSIONED DUMMY VARIABLES                                    FMFP 720
      DIMENSION H(1),X(1),G(1)                                          FMFP 730
C                                                                       FMFP 740
C        COMPUTE FUNCTION VALUE AND GRADIENT VECTOR FOR INITIAL ARGUMENTFMFP 750
      CALL FUNCT(N,X,F,G)                                               FMFP 760
C                                                                       FMFP 770
C        RESET ITERATION COUNTER AND GENERATE IDENTITY MATRIX           FMFP 780
      IER=0                                                             FMFP 790
      KOUNT=0                                                           FMFP 800
      N2=N+N                                                            FMFP 810
      N3=N2+N                                                           FMFP 820
      N31=N3+1                                                          FMFP 830
    1 K=N31                                                             FMFP 840
      DO 4 J=1,N                                                        FMFP 850
      H(K)=1.                                                           FMFP 860
      NJ=N-J                                                            FMFP 870
      IF(NJ)5,5,2                                                       FMFP 880
    2 DO 3 L=1,NJ                                                       FMFP 890
      KL=K+L                                                            FMFP 900
    3 H(KL)=0.                                                          FMFP 910
    4 K=KL+1                                                            FMFP 920
C                                                                       FMFP 930
C        START ITERATION LOOP                                           FMFP 940
    5 KOUNT=KOUNT +1                                                    FMFP 950
C                                                                       FMFP 960
C        SAVE FUNCTION VALUE, ARGUMENT VECTOR AND GRADIENT VECTOR       FMFP 970
      OLDF=F                                                            FMFP 980
      DO 9 J=1,N                                                        FMFP 990
      K=N+J                                                             FMFP1000
      H(K)=G(J)                                                         FMFP1010
      K=K+N                                                             FMFP1020
      H(K)=X(J)                                                         FMFP1030
C                                                                       FMFP1040
C        DETERMINE DIRECTION VECTOR H                                   FMFP1050
      K=J+N3                                                            FMFP1060
      T=0.                                                              FMFP1070
      DO 8 L=1,N                                                        FMFP1080
      T=T-G(L)*H(K)                                                     FMFP1090
      IF(L-J)6,7,7                                                      FMFP1100
    6 K=K+N-L                                                           FMFP1110
      GO TO 8                                                           FMFP1120
    7 K=K+1                                                             FMFP1130
    8 CONTINUE                                                          FMFP1140
    9 H(J)=T                                                            FMFP1150
C                                                                       FMFP1160
C        CHECK WHETHER FUNCTION WILL DECREASE STEPPING ALONG H.         FMFP1170
      DY=0.                                                             FMFP1180
      HNRM=0.                                                           FMFP1190
      GNRM=0.                                                           FMFP1200
```

```
      C                                                                 FMFP1210
      C        CALCULATE DIRECTIONAL DERIVATIVE AND TESTVALUES FOR DIRECTION FMFP1220
      C        VECTOR H AND GRADIENT VECTOR G.                          FMFP1230
           DO 10 J=1,N                                                  FMFP1240
           HNRM=HNRM+ABS(H(J))                                          FMFP1250
           GNRM=GNRM+ABS(G(J))                                          FMFP1260
        10 DY=DY+H(J)*G(J)                                              FMFP1270
      C                                                                 FMFP1280
      C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DIRECTIONAL FMFP1290
      C        DERIVATIVE APPEARS TO BE POSITIVE OR ZERO.               FMFP1300
           IF(DY)11,51,51                                               FMFP1310
      C                                                                 FMFP1320
      C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DIRECTION FMFP1330
      C        VECTOR H IS SMALL COMPARED TO GRADIENT VECTOR G.         FMFP1340
        11 IF(HNRM/GNRM-EPS)51,51,12                                    FMFP1350
      C                                                                 FMFP1360
      C        SEARCH MINIMUM ALONG DIRECTION H                         FMFP1370
      C                                                                 FMFP1380
      C        SEARCH ALONG H FOR POSITIVE DIRECTIONAL DERIVATIVE       FMFP1390
        12 FY=F                                                         FMFP1400
           ALFA=2.*(EST-F)/DY                                           FMFP1410
           AMBDA=1.                                                     FMFP1420
      C                                                                 FMFP1430
      C        USE ESTIMATE FOR STEPSIZE ONLY IF IT IS POSITIVE AND LESS THAN FMFP1440
      C        1. OTHERWISE TAKE 1. AS STEPSIZE                         FMFP1450
           IF(ALFA)15,15,13                                             FMFP1460
        13 IF(ALFA-AMBDA)14,15,15                                       FMFP1470
        14 AMBDA=ALFA                                                   FMFP1480
        15 ALFA=0.                                                      FMFP1490
      C                                                                 FMFP1500
      C        SAVE FUNCTION AND DERIVATIVE VALUES FOR OLD ARGUMENT     FMFP1510
        16 FX=FY                                                        FMFP1520
           DX=DY                                                        FMFP1530
      C                                                                 FMFP1540
      C        STEP ARGUMENT ALONG H                                    FMFP1550
           DO 17 I=1,N                                                  FMFP1560
        17 X(I)=X(I)+AMBDA*H(I)                                         FMFP1570
      C                                                                 FMFP1580
      C        COMPUTE FUNCTION VALUE AND GRADIENT FOR NEW ARGUMENT     FMFP1590
           CALL FUNCT(N,X,F,G)                                          FMFP1600
           FY=F                                                         FMFP1610
      C                                                                 FMFP1620
      C        COMPUTE DIRECTIONAL DERIVATIVE DY FOR NEW ARGUMENT.  TERMINATE FMFP1630
      C        SEARCH, IF DY IS POSITIVE. IF DY IS ZERO THE MINIMUM IS FOUND FMFP1640
           DY=0.                                                        FMFP1650
           DO 18 I=1,N                                                  FMFP1660
        18 DY=DY+G(I)*H(I)                                              FMFP1670
           IF(DY)19,36,22                                               FMFP1680
      C                                                                 FMFP1690
      C        TERMINATE SEARCH ALSO IF THE FUNCTION VALUE INDICATES THAT FMFP1700
      C        A MINIMUM HAS BEEN PASSED                                FMFP1710
        19 IF(FY-FX)20,22,22                                            FMFP1720
      C                                                                 FMFP1730
      C        REPEAT SEARCH AND DOUBLE STEPSIZE FOR FURTHER SEARCHES   FMFP1740
        20 AMBDA=AMBDA+ALFA                                             FMFP1750
           ALFA=AMBDA                                                   FMFP1760
      C        END OF SEARCH LOOP                                       FMFP1770
      C                                                                 FMFP1780
      C        TERMINATE IF THE CHANGE IN ARGUMENT GETS VERY LARGE      FMFP1790
           IF(HNRM*AMBDA-1.E10)16,16,21                                 FMFP1800
```

```
C                                                                       FMFP1810
C        LINEAR SEARCH TECHNIQUE INDICATES THAT NO MINIMUM EXISTS       FMFP1820
   21 IER=2                                                             FMFP1830
      RETURN                                                            FMFP1840
C                                                                       FMFP1850
C        INTERPOLATE CUBICALLY IN THE INTERVAL DEFINED BY THE SEARCH    FMFP1860
C        ABOVE AND COMPUTE THE ARGUMENT X FOR WHICH THE INTERPOLATION   FMFP1870
C        POLYNOMIAL IS MINIMIZED                                        FMFP1880
   22 T=0.                                                              FMFP1890
   23 IF(AMBDA)24,36,24                                                 FMFP1900
   24 Z=3.*(FX-FY)/AMBDA+DX+DY                                          FMFP1910
      ALFA=AMAX1(ABS(Z),ABS(DX),ABS(DY))                                FMFP1920
      DALFA=Z/ALFA                                                      FMFP1930
      DALFA=DALFA*DALFA-DX/ALFA*DY/ALFA                                 FMFP1940
      IF(DALFA)51,25,25                                                 FMFP1950
   25 W=ALFA*SQRT(DALFA)                                                FMFP1960
      ALFA=DY-DX+W+W
      IF (ALFA) 250,251,250
  250 ALFA=(DY-Z+W)/ALFA
      GO TO 252
  251 ALFA=(Z+DY-W)/(Z+DX+Z+DY)
  252 ALFA=ALFA*AMBDA
      DO 26 I=1,N                                                       FMFP1980
   26 X(I)=X(I)+(T-ALFA)*H(I)                                           FMFP1990
C                                                                       FMFP2000
C        TERMINATE, IF THE VALUE OF THE ACTUAL FUNCTION AT X IS LESS    FMFP2010
C        THAN THE FUNCTION VALUES AT THE INTERVAL ENDS. OTHERWISE REDUCEFMFP2020
C        THE INTERVAL BY CHOOSING ONE END-POINT EQUAL TO X AND REPEAT   FMFP2030
C        THE INTERPOLATION. WHICH END-POINT IS CHOOSEN DEPENDS ON THE   FMFP2040
C        VALUE OF THE FUNCTION AND ITS GRADIENT AT X                    FMFP2050
C                                                                       FMFP2060
      CALL FUNCT(N,X,F,G)                                               FMFP2070
      IF(F-FX)27,27,28                                                  FMFP2080
   27 IF(F-FY)36,36,28                                                  FMFP2090
   28 DALFA=0.                                                          FMFP2100
      DO 29 I=1,N                                                       FMFP2110
   29 DALFA=DALFA+G(I)*H(I)                                             FMFP2120
      IF(DALFA)30,33,33                                                 FMFP2130
   30 IF(F-FX)32,31,33                                                  FMFP2140
   31 IF(DX-DALFA)32,36,32                                              FMFP2150
   32 FX=F                                                              FMFP2160
      DX=DALFA                                                          FMFP2170
      T=ALFA                                                            FMFP2180
      AMBDA=ALFA                                                        FMFP2190
      GO TO 23                                                          FMFP2200
   33 IF(FY-F)35,34,35                                                  FMFP2210
   34 IF(DY-DALFA)35,36,35                                              FMFP2220
   35 FY=F                                                              FMFP2230
      DY=DALFA                                                          FMFP2240
      AMBDA=AMBDA-ALFA                                                  FMFP2250
      GO TO 22                                                          FMFP2260
C                                                                       FMFP2270
C        TERMINATE, IF FUNCTION HAS NOT DECREASED DURING LAST ITERATION
   36 IF (OLDF-F+EPS) 51,38,38
C
C        COMPUTE DIFFERENCE VECTORS OF ARGUMENT AND GRADIENT FROM
C           TWO CONSECUTIVE ITERATIONS
   38 DO 37 J=1,N
      K=N+J
      H(K)=G(J)-H(K)
```

```
      K=N+K
   37 H(K)=Y(J)-H(K)
C                                                                       FMFP2380
C        TEST LENGTH OF ARGUMENT DIFFERENCE VECTOR AND DIRECTION VECTOR FMFP2390
C        IF AT LEAST N ITERATIONS HAVE BEEN EXECUTED. TERMINATE, IF     FMFP2400
C        BOTH ARE LESS THAN  EPS                                        FMFP2410
      IFR=0
      IF(KOUNT-N)42,39,39                                               FMFP2430
   39 T=0.                                                              FMFP2440
      Z=0.                                                              FMFP2450
      DO 40 J=1,N                                                       FMFP2460
      K=N+J                                                             FMFP2470
      W=H(K)                                                            FMFP2480
      K=K+N                                                             FMFP2490
      T=T+ABS(H(K))                                                     FMFP2500
   40 Z=Z+W*H(K)                                                        FMFP2510
      IF(HNRM-EPS)41,41,42                                              FMFP2520
   41 IF(T-EPS)56,56,42                                                 FMFP2530
C                                                                       FMFP2540
C        TERMINATE, IF NUMBER OF ITERATIONS WOULD EXCEED  LIMIT         FMFP2550
   42 IF(KOUNT-LIMIT)43,50,50                                           FMFP2560
C                                                                       FMFP2570
C        PREPARE UPDATING OF MATRIX H                                   FMFP2580
   43 ALFA=0.                                                           FMFP2590
      DO 47 J=1,N                                                       FMFP2600
      K=J+N3                                                            FMFP2610
      W=0.                                                              FMFP2620
      DO 46 L=1,N                                                       FMFP2630
      KL=N+L                                                            FMFP2640
      W=W+H(KL)*H(K)                                                    FMFP2650
      IF(L-J)44,45,45                                                   FMFP2660
   44 K=K+N-L                                                           FMFP2670
      GO TO 46                                                          FMFP2680
   45 K=K+1                                                             FMFP2690
   46 CONTINUE                                                          FMFP2700
      K=N+J                                                             FMFP2710
      ALFA=ALFA+W*H(K)                                                  FMFP2720
   47 H(J)=W                                                            FMFP2730
C                                                                       FMFP2740
C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF RESULTS      FMFP2750
C        ARE NOT SATISFACTORY                                           FMFP2760
      IF(Z*ALFA)48,1,48                                                 FMFP2770
C                                                                       FMFP2780
C        UPDATE MATRIX H                                                FMFP2790
   48 K=N31                                                             FMFP2800
      DO 49 L=1,N                                                       FMFP2810
      KL=N2+L                                                           FMFP2820
      DO 49 J=L,N                                                       FMFP2830
      NJ=N2+J                                                           FMFP2840
      H(K)=H(K)+H(KL)*H(NJ)/Z-H(L)*H(J)/ALFA                            FMFP2850
   49 K=K+1                                                             FMFP2860
      GO TO 5                                                           FMFP2870
C        END OF ITERATION LOOP                                          FMFP2880
C                                                                       FMFP2890
C        NO CONVERGENCE AFTER  LIMIT  ITERATIONS                        FMFP2900
   50 IFR=1                                                             FMFP2910
      RETURN                                                            FMFP2920
C                                                                       FMFP2930
C        RESTORE OLD VALUES OF FUNCTION AND ARGUMENTS                   FMFP2940
   51 DO 52 J=1,N                                                       FMFP2950
```

```
      K=N2+J                                                            FMFP2960
   52 X(J)=H(K)                                                         FMFP2970
      CALL FUNCT(N,X,F,G)                                               FMFP2980
C                                                                       FMFP2990
C        REPEAT SEARCH IN DIRECTION OF STEEPEST DESCENT IF DERIVATIVE   FMFP3000
C        FAILS TO BE SUFFICIENTLY SMALL                                 FMFP3010
      IF(GNRM-EPS)55,55,53                                              FMFP3020
C                                                                       FMFP3030
C        TEST FOR REPEATED FAILURE OF ITERATION                         FMFP3040
   53 IF(IER)56,54,54                                                   FMFP3050
   54 IER=-1                                                            FMFP3060
      GOTO 1                                                            FMFP3070
   55 IER=0                                                             FMFP3080
   56 RETURN                                                            FMFP3090
      END                                                               FMFP3100
END OF FILE
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